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TO: Tamthom Troung Location: REM/5C18

Art Unit: 1624

Friday, June 24, 2005

Case Serial Number: 09/918039

From: Mary Hale

Location: Biotech/Chem Library

Rem 1D86 Phone: 2-2507

Mary.Hale@uspto.gov

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Name: TAMTHOM TRUONG	•		图 思
Employee Number: 74142 Phone: X20676	T .		
Art Unit or Office: 1624 Building & Room Number: REM – 5C18		<u>;</u>	
Enter the case serial number (Required): 9/918,039 If not related to a patent application, please enter NA here.	•		
Class / Subclass(es) 514/300; 546/113			
Earliest Priority Filing Date: 12/13/1996	:62		478.76
Format preferred for results: Paper Diskette E-mail	:62 :48_58		
Provide detailed information on your search topic:	14		

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• FAX or send the abstract, pertinent claims (not all of the claims), drawings, or chemical structures to your EIC or branch library.

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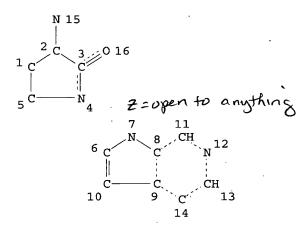
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L1 STR

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE L2 STR



NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE L3 STR

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L5 52 SEA FILE=REGISTRY SSS FUL L1 OR L2 OR L3

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SEARCH TIME: 00.00.02

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Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

This file contains CAS Registry Numbers for easy and accurate substance identification.

L6 10 L5

=> d 1-10 ibib abs hitstr

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

Ld ANSWER 1 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:832890 CAPLUS
COMMAN NUMBER: 1142:19473
TITLE: Comparing Ligand Interactions with Multiple Receptors via Serial Docking
AUTHOR(S): Fernandes, Miguel X.; Kairys, Visvaldas; Gilson, Michael X.
CORPORATE SOURCE: Center for Advanced Research in Biotechnology, U. Maryland Biotechnology Institute, Rockville, MD, 20850, USA
SOURCE: Journal of Chemical Information and Computer Sciences (2004), 44(6), 1961-1970
CODEN: JCISDS: ISSN: 0095-2338
American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: Bright
AB Standard uses of ligand-receptor docking typically focus on the association of candidate ligands with a single targeted receptor, but actual applications increasingly require comparisons across multiple receptors can help to gardet homol. models for virtual compound screening and to discover ligands
that bind to one set of receptors but not to another, potentially similar, set. A serial docking algorithm is furthermore described that reduces the Computational costs of such calcans. by testing compds. against a series

computational costs of such calcns. by testing compds. against a series

receptor structures and discarding a compound as soon as it fails to satisfy
specified bind/no bind criteria for each receptor. The algorithm also realizes substantial efficiencies by taking advantage of the fact that a ligand typically binds in similar conformations to similar receptors. Thus, once detailed docking has been used to fit a ligand into the first of a series of similar receptors, much less extensive calcns. can be used for the remaining structures.

IT 209265-84-7, RPR 208707
RL. BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(ligand interactions with multiple receptors via serial docking through

ugn electrostatic force and van der Waals forces)
209285-84-7 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 1 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT: THIS

FORMAT

THERE ARE 58 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

$$\begin{array}{c|c}
 & CH & CH_2 - N & N - SO_2 & CH & S \\
\hline
 & CH & S & C1
\end{array}$$

The discovery and SAR of ketopiperazino methylazaindole factor Xa inhibitors are described. Structure-activity data suggesting that this class of inhibitors does not bind in the canonical mode were confirmed by an X-ray crystal structure showing the neutral haloarom. bound in the SI subsite. The most potent azaindole (I, RPR209685) is selective against related serine proteases and attains higher levels of exposure upon oral dosing than comparable benzamidines and benzamidine isosteres. Compound

was efficacious in the canine AV model of thrombosis 209285-75-6 209285-82-5

RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

study)

(discovery of an orally efficacious inhibitor of coagulation factor Xa which incorporates a neutral Pl ligand)

RN 209285-75-6 CAPIUS

CN Benzo[b]thiophene-2-sulfonamide,
6-chloro-N-[[35]-2-coo-1-(1H-pytrolo[3],2-c)
c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

209285-82-5 CAPLUS RN 209285-82-5 CAPLUS
CN Benzo(b) Ethophene-2-sulfonamide,
6-chloro-N-[(3S)-2-oxo-1-{lH-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) {CA INDEX NAME}

Absolute stereochemistry.

REFERENCE COUNT:

16

THERE ARE 16 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2002:894400 CAPLUS DOCUMENT NUMBER: 138:133092 Crystal Structures of Two Pote Inhibitors

Crystal Structures of Two Potent Nonamidine

Bound to Factor Xa Adler, Marc; Kochanny, Monica J.; Ye, Bin; Rumennik, Galina; Light, David R.; Biancalana, Sara; Whitlow, Marc

CORPORATE SOURCE:
SOURCE:
SOURCE:
Berlex Biosciences, Richmond, CA, 94804-0099, USA
Biochemistry (2002), 41(52), 15514-15523
CODEN: BICKHW; ISSN: 0006-2960

American Chemical Society
DOCUMENT TYPE:
Journal
LANGUAGE:
English
AB There has been intense interest in the development of factor Xa inhibitors

inhibitors inhibitors treatment of thrombotic diseases. Our laboratory has developed

ries of novel non-amidine inhibitors of factor Xa. This paper presents two crystal structures of compds. from this series bound to factor Xa. The first structure is derived from the complex formed between factor Xa and compound 1. Compound 1 was the first non-amidine factor Xa inhibitor

from Our laboratory that had measurable potency in an in vitro assay of

coagulant activity. The second compound, 2, has a molar affinity for factor Xa (Kiapp) of 7 pM and good bioavailability. The two inhibitors bind in an L-shaped conformation with a chloroarom, ring buried deeply in the Sl pocket. The opposite end of these compds. contains a basic substituent that extends into the S4 binding site. A chlorinated Ph ring bridges the substituents in the S1 and S4 pockets via amide linkers. The overall conformation is similar to the previously published structures for amidine-based inhibitors complexed with factor Xa. However, there are significant differences in the interactions between the inhibitor and the protein at the atomic level. Most notably, there is no group that forms

salt bridge with the carboxylic acid at the base of the S1 pocket (Asp189). Each inhibitor forms only one well-defined hydrogen bond to

protein. There are no direct charge-charge interactions. The results indicate that electrostatic interactions play a secondary role in the binding of these potent inhibitors.

193285-84-7, RPR-2087079,
RM: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(structure-activity relationship of factor Xa inhibitors; crystal structure-activity relationship of factor Xa inhibitors crystal structures of two potent nonamidine inhibitors bound to factor Xa) 209285-84-7 CAPLUS

Thieno [3, 2-b] pyridine-2-sulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:630893 CAPLUS DOCUMENT NUMBER: 135:195505

TITLE: Preparation of azaheterocyclic sulfonamides as factor Xa inhibitors

INVENTOR(S):

Am infinitors
Choi-Sledeski, Yong Mi; Pauls, Heinz W.; Barton,
Jeffrey N.; Ewing, William R.; Green, Daniel M.;
Becker, Michael R.; Gong, Yong; Levell, Julian
Aventis Pharma Deutschland GmbH, Germany PATENT ASSIGNEE(S):

SOURCE: U.S., 96 pp., Cont.-in-part of U.S. Ser. No. 90,492. CODEN: USXXAM

DOCUMENT TYPE: Patent

FAMILY ACC. NUM. COUNT:

PATENT INFORMATI	ON:			
PATENT NO.			APPLICATION NO.	
			US 1999-453307	
US 6281227	B1		WO 1997-US22406	19991202
WO 9825611				
			BG, BR, BY, CA, CN,	
			IL, IS, JP, KE, KG,	
			MG, MK, MN, MW, MX,	
			SL, TJ, TM, TR, TT,	UA, UG, US, UZ,
			KZ, MD, RU, TJ, TM	
			ZW, AT, BE, CH, DE,	
			PT, SE, BF, BJ, CF,	CG, CI, CM, GA,
GN,	ML, MR, NE,			
US 6602864			US 1998-90492	19980603
WO 9962904			WO 1999-US12312	
			BG, BR, BY, CA, CN,	
			IL, IS, JP, KE, KG,	
LK,	LR, LS, LT,	LU, LV, MD,	MG, MK, MN, MW, MX,	NO, NZ, PL, PT,
RO,	RU, SD, SE,	SG, SI, SK,	SL, TJ, TM, TR, TT,	UA, UG, US, UZ,
VN,	YU, ZW, AM,	AZ, BY, KG,	KZ, MD, RU, TJ, TM	
RW: GH,	GM, KE, LS,	MW, SD, SL,	SZ, UG, ZW, AT, BE,	CH, CY, DE, DK,
ES,	FI, FR, GB,	GR, IE, IT,	LU, MC, NL, PT, SE,	BF, BJ, CF, CG,
CI,	CM, GA, GN,	GW, ML, MR,	NE, SN, TD, TG	
WO 20010397	59 A2	20010607	WO 2000-EP11577	20001121
WO 20010397	59 A3	20020117		
W: AE,	AG, AL, AM,	AT, AU, AZ,	BA, BB, BG, BR, BY,	BZ, CA, CH, CN,
CR,	CU, CZ, DE,	DK, DM, DZ,	EE, ES, FI, GB, GD,	GE, GH, GM, HR,
HU.	ID. IL. IN.	IS. JP. KE.	KG, KP, KR, KZ, LC,	LK. LR. LS. LT.
			MW, MX, MZ, NO, NZ,	
			TM, TR, TT, TZ, UA,	
			MD, RU, TJ, TM	,
			SL, SZ, TZ, UG, ZW,	AT. BE. CH. CY.
			IE, IT, LU, MC, NL,	
			GW, ML, MR, NE, SN,	
US 20020133			US 2001-918039	
PRIORITY APPLN.			US 1996-33159P	P 19961213
			•	
			WO 1997-US22406	A2 19971203
			US 1998-90492	A2 19980603
			WO 1999-US12312	A2 19990603
			US 1999-453307	A 19991202

L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

THERE ARE 30 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) OTHER SOURCE(S): MARPAT 135:195505

Title compds. [I; X = (CHR3)m; R = (un)substituted heteroaryl; R1, R2 =

(un)substituted alkyl, alkenyl, aralkyl; R3 = H, OH, (un)substituted alkyl, aryl, heteroaryl; R4 = H, (un)substituted alkyl, aryl, aralkyl;

R6 - H; R5R6 - O; R7, R8 - H, (un)substituted alkyl, aryl, aralkyl, heteroaryl; R7R8 - O; R3R7 - alkylene; m - 0-3] were prepared Thus, title

compound II was prepared from 3-acetamido-4-methylbenzaldehyde, malonic acid,

and 7-methoxy-2-naphthalenesulfonyl chloride in 10 steps. II had a Ki of 80 nM for inhibition of factor Ka. 203266-49-72 203286-51-12 203286-82-82 203286-93-92 203286-84-02 203287-05-82 233336-10-02 233336-17-12 233336-18-29

251936-22-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (preparation of azaheterocyclic sulfonamides as inhibitors of factor

209286-49-7 CAPLUS
Carbamic acid, [(3S)-2-oxo-1-{2-(1H-pyrrolo[3,2-c]pyridin-1-yl)ethyl]-3-pyrrolidinyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

209286-51-1 CAPLUS
2-Pyrrolidinone, 3-amino-1-{2-(1H-pyrrolo{3,2-c]pyridin-1-yl}ethyl}-,

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (3S)-, monoacetate (9CI) (CA INDEX NAME) (Continued)

CM 1

CRN 209286-50-0 CMF C13 H16 N4 O

Absolute stereochemistry

2

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209286-82-8 CAPLUS Carbamic acid, {(3S)-1-[[4-chloro-1-(phenylsulfonyl)-1H-pyrrolo[3,2-c]pyridin-2-yl]methyl]-2-oxo-3-pyrrolidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 209286-83-9 CAPLUS
CN 1H-Pyrrolo(3,2-c)pyridine,
2-[([38)-3-amino-2-oxo-1-pyrrolidiny1]methy1]-4chloro-1-(phenylsulfony1)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251936-16-0 CAPLUS

231336-16-0 CAPMUS
HI-Pyrrolo(3,2-c)pyridine-1-carboxylic acid, 2-[[(3S)-2-oxo-3[{(phenylmethoxy)carbonyl]amino]-1-pyrrolidinyl]methyl}-,
1,-dimethylethyl ester (9C1) (CA INDEX NAME)

Absolute stereochemistry

251936-17-1 CAPLUS
1H-Pyrrolo[3,2-c]pyridine-1-carboxylic acid, 2-[[(3S)-3-amino-2-oxo-1-pyrrolidinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251936-18-2 CAPLUS
CN 1H-Pyrrolo[3,2-c]pyridine-1-carboxylic acid,
2-[[(3S)-3-[[(5'-chloro]2,2'-bithiophen]-5-yl)sulfonyl]amino]-2-oxo-1-pyrrolidinyl]methyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

• HC1

209286-84-0 CAPLUS
Benzo[b]thiophene-2-sulfonamide, 6-chloro-N-[(3S)-1-[[4-chloro-1-(pheny]sulfony]]-1H-pyrrolo[3,2-c]pyridin-2-yl]methyl]-2-oxo-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

209287-05-8 CAPLUS
1H-Pyrrolo[2,3-c]pyridine-1-carboxylic acid, 2-[[(3S)-3-[[(6-chlorobenzo[b]thien-2-yl)sulfonyl]amino]-2-oxo-1-pyrrolidinyl]methyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

Absolute stereochemistry

251936-22-8 CAPLUS
IH-Pyrrolo[3,2-c]pyridine-1-carboxylic acid, 2-{{(38}-3-{{(2-(5-chloro-2-thieny)|sulfonyl]amino]-2-oxo-1-pyrrolidinyl]methyl}-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown

209285-47-2P 209285-74-5P 209285-75-6P
209285-82-59 209285-83-6P 209285-84-7P
209285-85-8P 251936-19-3P 251936-23-9P
251937-86-6P 251937-86-7P 251937-97-8P
251937-86-9P 251937-89-0P 251937-90-3P
251937-91-4P 251937-93-1P 251937-93-6P
251937-91-7P 251937-96-1P 251937-93-6P
251937-91-7P 251937-96-1P 251937-99-2P
251938-00-8P 251938-01-9P 251938-02-0P
251938-00-8P 251938-01-9P 251938-03-3P
251938-06-4P 251938-38-2P 251938-39-3P
251938-46-2P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological Study); PREP (Preparation); USES (Usen)
(preparation of azaheterocyclic sulfonamides as inhibitors of factor

209285-47-2 CAPLUS
2-Naphthalenesulfonamide, 7-methoxy-N-[(3S)-2-oxo-1-[2-(1H-pyrrolo[3,2-c]pyridin-1-yl)ethyl]-3-pyrrolidinyl]-, mono(trifluoroacetate) (9CI) | INDEX RAME)

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CH 2

CRN 76-05-1

RN 209285-74-5 CAPLUS
CN Benzo(b)thiophene-2-sulfonamide, 6-chloro-N-[(3S)-1-[(4-chloro-1H-pyrrolo[3,2-c]pyridin-2-y1)methyl)-2-oxo-3-pyrrolidinyl]- (9CI) (CA INDEX

Absolute stereochemistry.

RN 209285-75-6 CAPLUS
CN Benzo[b]thiophene-2-sulfonamide,
6-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) CM 1

CRN 209285-82-5 CMF C20 H17 C1 N4 O3 S2

Absolute stereochemistry.

CM 2 CRN 76-05-1 CMF C2 H F3 O2

RN 209285-84-7 CAPLUS
CN Thieno{3,2-b}pyridine-2-sulfonamide, N-{(3S)-2-oxo-1-(1H-pyrrolo[2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) c}pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 209285-82-5 CAPLUS
CN Benzo[b]thiophene-2-sulfonamide,
6-chloro-N-[(35)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 209285-83-6 CAPLUS
CN Benzo[b]thiophene-2-sulfonamide,
6-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3c]pyridin-2-ylmethyl)-3-pyrrolidinyl]-, mono(trifluoroacetate) [9CI] (CA
INDEX NAME)

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 209285-85-8 CAPLUS
CN Thieno[3,2-b]pyridine-2-sulfonamide, N-[(35)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209285-84-7 CMF C19 H17 N5 03 S2

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 O2 L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251936-19-3 CAPLUS
[2,2'-Bithiophene]-5-sulfonamide, 5'-chloro-N-{(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251936-23-9 CAPLUS
CN Ethenesulfonamide,
2-(5-chloro-2-thienyl)-N-((3S)-2-cxo-1-(1H-pyrrolo[3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]: (9CI) (CA INDEX NAME)

251937-85-6 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, N-{(3S)-2-oxo-1-{1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9Cf) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251937-88-9 CAPLUS
Thieno[2,3-b]pyridine-2-sulfonamide, N-{(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251937-89-0 CAPLUS
2-Thiophenesulfonamide, 5-(3-isoxazolyl)-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251937-86-7 CAPLUS
2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl}-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251937-87-8 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, 5-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251937-90-3 CAPLUS
Thieno{2,3-b}pyridine-2-sulfonamide, 6-chloro-N-{{35}-2-oxo-1-{1H-pyrrolo[3,2-c]pyridin-2-ylmethyl}-3-pyrrolidinyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251937-91-4 CAPLUS
CN Benzenesulfonamide,
4-(1,1-dmethylethyl)-N-{(3s)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry

251937-92-5 CAPLUS
Thieno[3,2-c]pyridine-2-sulfonamide, 4-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251937-93-6 CAPLUS
2-Thiophenesulfonamide, N-{(3S)-2-oxo-1-{1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl}-5-(4-pyridinyl)- {9Cl} (CA INDEX NAME)

Absolute stereochemistry.

251937-94-7 CAPLUS
Benzo[b]thiophene-2-sulfonamide, 5-chloro-3-methyl-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251937-97-0 CAPLUS
2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

251937-98-1 CAPLUS
Thieno(3,2-b)pyridine-2-sulfonamide, 5-chloro-N-[(35)-2-oxo-1-(1H-pyrrolof2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyll- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251937-95-8 CAPLUS

Thieno(2,3-c)pyridine-2-sulfonamide, 7-chloro-N-((35)-2-oxo-1-(1H-pyrrolo(3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251937-96-9 CAPLUS 1H-Benzimidazole-2-sulfonamide, 5-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251937-99-2 CAPLUS
Thieno [2,3-b]pyridine-2-sulfonamide, N-{(3S)-2-oxo-1-(1H-pyrrolo(2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251938-00-8 CAPLUS
2-Thiopheneaulfonamide, 5-(3-isoxazolyl)-N-((3S)-2-oxo-1-(1H-pyrrolo[2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

251938-01-9 CAPLUS Thieno[2,3-b]pyridine-2-sulfonamide, 6-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251938-02-0 CAPLUS
[2,2'-Bithiophene]-5-sulfonamide, 5'-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251938-03-1 CAPLUS
CN Benzenesulfonamide,
4-(1,1-damethylethyl)-N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251938-04-2 CAPLUS
Thieno[3,2-c]pyridine-2-sulfonamide, 4-chloro-N-((3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251938-07-5 CAPLUS
Thieno[2,3-c]pyridine-2-sulfonamide, 7-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo{2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251938-08-6 CAPLUS HH-Benzimidazole-2-sulfonamide, 5-chloro-N-{(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) Absolute stereochemistry.

251938-05-3 CAPLUS
2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Benzo[b]thiophene-2-sulfonamide, 5-chloro-3-methyl-N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251938-35-9 CAPLUS
2-Pyrrolidinone, 1-[(4-amino-7-quinazolinyl)methyl]-3-[(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)amino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251938-38-2 CAPLUS
CN Etheneaulfonamide,
2-(5-chloro-2-thienyl)-N-[(3R)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown

251938-39-3 CAPLUS Glycine. N-[[2-(5-chloro-2-thienyl)ethenyl]sulfonyl]-N-[(3R)-2-oxo-1-(1H-pyrrolol3,2-cl)pyridin-2-ylmethyl]-3-pyrrololidinyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Absolute stereochemistry.
Double bond geometry unknown

251938-46-2 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, N-[(3R)-2-oxo-1-(1H-pyrrolo[2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 251938-45-1 CMF C19 H17 N5 O3 S2

Absolute stereochemistry.

2 76-05-1 C2 H F3 O2

СМ

L6 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:416785 CAPLUS
DOCUMENT NUMBER: 15:46082
TITLE: Preparation of
N-(oxopyrrolidinyl)naphthalenesulfonami
des and analogs as factor Xa inhibitors
(Choi-Sledeski, Yong Mi; Pauls, Heinz W.; Barton,
Jeffrey N.; Ewing, William R.; Green, Daniel M.;
Becker, Michael R.; Gong, Yong; Levell, Julian
Aventis Pharma Deutschland G.m.b.H., Germany
POT Int. Appl., 106 pp.
COODE: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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	WO	2001	0397	59		A3		2002	0117									
		W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ĐΖ,	CA,	CH,	CN,
			CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR.
			HU,	ID.	IL.	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT.
			LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO.	NZ,	PL,	PT,	RO,	RU,
			SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	UZ.	VN,	YU,
			ZA,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ.	TM					
		RW:	GH,	GM,	ΚĒ,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG.	ZW,	ΑŤ,	BE.	CH,	CY,
			DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
			BJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
	US	6281	227			B1		2001	0828	1	US 1	999-	4533	07		1	9991	202
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										1	US 1	996-	3315	9 P		P 1	9961	213
										,	WO 1	997-1	J522	406		A2 1	9971	203
										,	US 1	998-	9049	2		A2 1	9980	603
										1	WO 1	999-1	US12	312		A2 1	9990	603

OTHER SOURCE(S):

MARPAT 135:46082

Title compds. [(un)substituted I; R = N-containing heteroaryl; R1 = H, (acyl)alkyl, (hetero)arylalkyl, etc.; R2 = H, (hetero)arylalkyl, etc.; Carbamoylalkyl, etc.; Z = (NH or NHO-orinterrupted or -terminated) alkylene; Z1 = (CH2)0-3] were prepared Thus, I (R1 = H, Z1 = CH2)(II; R

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

(Continued)

FORMAT

L6 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
H, R2 = CO2cMe3, Z = bond) was N-alkylated by 7-bromomethyl-1chloroisoquinoline (prepn. each given) and the deprotected product
N-acylated by 7-methoxynaphthalene-2-sulfonyl chloride (prepn. given) to
give, in 2 addn1 steps, II (R = 1-amino-7-isoquinobyl, R2 =
7-methoxynaphthalene-2-sulfonyl, Z = CH2). Data for biol. activity of I
were given.
IT 203285-47-2P
RL BAC (Biological activity or effector, except adverse); BSU
(Biological
Study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-(oxopyrrolidinyl) naphthalenesulfonamides and
analogs as
factor Xa inhibitors)
RN 209285-47-2 CAPLUS
CN 2-Maphthalenesulfonamide, 7-methoxy-N-[{3S}-2-oxo-1-{2-(1H-pyrrolo[3,2-c]pyridin-1-yl)ethyl}-3-pyrrolidinyl}-, mono(trifluoroacetate) (9CI) (CA
INDEX NAME)

2

CO2H

IT 209286-49-7P 209286-50-0P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(Reactant or reagent)
(Preparation of N-(oxopyrrolidinyl))naphthalenesul(onamides and analogs as factor Xs inhibitors)
RN 209286-49-7 CAPLUS
CN Carbamic acid, ([35]:2-oxo-1-[2-(1H-pyrrolo[3,2-c]pyridin-1-yl)ethyl]-3-pyrrolidinyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

L6 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2005 ACS On STN Absolute stereochemistry. (Continued)

209286-50-0 CAPLUS 2-Pyrrolidinone, 3-amino-1-[2-(1H-pyrrolo[3,2-c]pyridin-1-yl)ethyl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

ANSWER 6 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT: THIS

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L6 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2000:543073 CAPLUS

DOCUMENT NUMBER: TITLE: 133:261091

Crystal Structures of Human Factor Xa Complexed with Potent Inhibitors Maignan, Sebastien; Guilloteau, Jean-Pierre;

AUTHOR (S) :

Pouzieux,

Stephanie; Choi-Sledeski, Yong Mi; Becker, Michael R.;

Klein, Scott I.; Ewing, William R.; Pauls, Henry W.; Spada, Alfred P.; Mikol, Vincent Department of Structural Biology, Aventis Pharma, Vitry/Seine, F-94403, Fr. Journal of Medicinal Chemistry (2000), 43(17), 1226-3232 CORPORATE SOURCE:

SOURCE:

J225-3232 CODEN: JMCMAR; ISSN: 0022-2623 American Chemical Society Journal PUBLISHER:

DOCUMENT TYPE: LANGUAGE: AB Involved

DOCUMENT TYPE: Journal English
LANGUAGE: English
BI Involved in the coagulation cascade, factor Xa (FXa) is a serine protease which has received great interest as a potential target for the development of new antithrombotics. Although there is a great wealth of structural data on thrombin complexes, few structures of ligand/FXa complexes have been reported, presumably because of the difficulty in growing crystals. Reproducible crystallization conditions for human des-folia-45

Clai-45

Coagulation FXa have been found. This has led to an improvement in the diffraction quality of the crystals (about 2.1 Å) when compared to the previously reported forms (2.3-2.8 Å) thus providing a suitable platform for a structure-based drug design approach. A series of cryst structures of noncovalent inhibitors complexed with FXa have been

three of which are presented herein. These include compds. containing

benzamidine moiety and surrogates of the basic group. The benzamidine-containing compound binds in a canonical fashion typical of synthetic serine protease inhibitors. On the contrary, mols. that

synthetic serine processe inhibitors. On the contrary, mols. that contain surrogates of the benzamidine group do not make direct hydrogen-bonding interactions with the carboxylate of Asp189 at the bottom of the S1 pocket. The structural data provide a likely explanation for the specificity of these inhibitors and a great aid in the design of bioavailable potent FXa inhibitors.

IT 209285-84-7, RPR 209707
RL: BAC (Biological activity or effector, except adverse); BPR (Biological study); PROC (Process) (Biological study); PROC (Process) (Biological study); PROC (Process) (Crystal structures of human factor Xa complexed with potent inhibitors)

RN 209285-84-7 CAPLUS
CN Thieno[3,2-b]pyridine-2-sulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:379659 CAPLUS

133:144473

AUTHOR(S): Solid-phase parallel synthesis of azarene pyrrolidinones as factor Xa inhibitors

GONG, Yong; Becker, Michael; Choi-sledeaki, Yong Mi; Davis, Roderick S.; Salvino, Joseph M.; Chu, Valeria; Brown, Karen D.; Pauls, Henry W.

CORPORATE SOURCE: Brown, Karen D.; Pauls, Henry W.

Department of Medicinal Chemistry, Rhone-Poulenc Rorer, Collegeville, PA, 19426, USA

Bioorganic & Medicinal Chemistry Letters (2000), 10(10, 1033-1036)

CODEN: BMCLE8; ISSN: 0960-894X

Elsevier Science Ltd.

LAMGUAGE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S):

English CASREACT 133:144473

A focused library (4+14) prepared from 4-aminopyridine and 4-, 5-, and 6-azoindole templates was synthesized using 14 polymer-supported 4-amido-2,3-5,6-textefluorophenyl (TFP) sulfonate esters and heteroarylmethyl-substituted arylsulfonylamino pyrrolidinones such as I

11

Several compds. were

heteroary/methyl-substituted arylsulfonylamino pyrrolidinones such as to give a library of factor Xa inhibitors such as II. Several compds. w identified as factor Xa inhibitors (ICSOSO.) µM) helping to establish the SAR among these four series of azarene pyrrolidinones. E.g., factor Xa was inhibited by II with a Ki of 15 nM.

17 209285-75-6P 209285-82-5P 209285-84-7P 251936-19-3P 251937-88-9P 251937-89-6-7P 251937-89-9P 251937-89-9P 251937-89-9P 251937-89-9P 251937-91-9P 251937-91-9P 251937-91-9P 251937-91-P 251937-91-P 251937-91-P 251937-91-P 251937-91-P 251937-91-P 251937-91-P 251937-91-P 251938-02-0P 251938-03-1P 251938-03-P 251938

L6 ANSMER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS ON STN (Contin RN 209285-75-6 CAPLUS CN Benzo(b)thiophene-2-sulfonamide, 6-chloro-N-{(35)-2-xox-1-(1H-pyrrolo[3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 209285-82-5 CAPLUS .
CN Benzo[b]thiophene-2-eulfonamide,
6-chloro-N-f(3S)-2-coxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

209285-84-7 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251937-86-7 CAPLUS
2-Thiophenesulfonamide, N-{{3S}-2-oxo-1-{1H-pyrrolo[3,2-c]pyridin-2-ylmethyl}-3-pyrrolidinyl}-5-{2-pyridinyl}- (9CI) (CA-INDEX NAME)

251937-87-8 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, 5-chloro-N-{(3S)-2-oxo-1-(1H-pyrrolo[3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251936-19-3 CAPLUS (2, 2'-Bithiophenel-5-sulfonamide, 5'-chloro-N-((35)-2-oxo-1-(1H-pyrroloid,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

251937-85-6 CAPLUS Thieno(3,2-b)pyridine-2-sulfonamide, N-[(3S)-2-0x0-1-(1H-pyrrolo(3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251937-88-9 CAPLUS

Thieno[2,3-b]pyridine-2-sulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251937-89-0 CAPLUS
2-Thiophenesulfonamide, 5-{3-isoxazolyl}-N-{{3S}-2-oxo-1-{1H-pyrrolo{3,2-c}pyridin-2-ylmethyl}-3-pyrrolidinyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251937-90-3 CAPLUS
Thieno[2,3-b]pyridine-2-sulfonamide, 6-chloro-N-{(3S)-2-oxo-1-{1H-pyrrolo[3,2-c]pyridin-2-ylmethyl}-3-pyrrolidinyl}- (9CI) (CA INDEX NAME)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 251937-91-4 CAPLUS
CN Benzenesulfonamide,
4-(1,1-dimethylethyl)-N-[(3S)-2-0x0-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251937-92-5 CAPLUS
Thieno[3,2-c]pyridine-2-sulfonamide, 4-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251937-95-8 CAPLUS
Thieno[2,3-c]pyridine-2-sulfonamide, 7-chloro-N-{(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251937-96-9 CAPLUS
'H-Benzimidazole-2-sulfonamide, 5-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251937-93-6 CAPLUS
2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]-5-(4-pyridinyl)- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

251937-94-7 CAPLUS
Benzo[b]thiophene-2-sulfonamide, 5-chloro-3-methyl-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251937-97-0 CAPLUS .
2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl}-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

251937-98-1 CAPLUS
Thieno(3,2-b)pyridine-2-sulfonamide, 5-chloro-N-[(35)-2-oxo-1-(1H-pyrrolo(2,3-e)pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251937-99-2 CAPLUS
Thieno[2,3-b]pyridine-2-sulfonamide, N-([35]-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-y|methyl]-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251938-00-8 CAPLUS
2-Thiophenesulfonamide, 5-{3-isoxazolyl}-N-{(35)-2-oxo-1-(1H-pyrrolo[2,3-c|pyridin-2-ylmethyl)-3-pyrrolidinyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251938-01-9 CAPLUS Thieno(2,3-b)pyridine-2-sulfonamide, 6-chloro-N-{(3S)-2-oxo-1-(1H-pyrrolo(2,3-c)pyridin-2-ylmethyl)-3-pyrrolodinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251938-05-3 CAPLUS
2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

251938-06-4 CAPLUS
Benzo[b]thiophene-2-sulfonamide, 5-chloro-3-methyl-N-[(3S)-2-oxo-1-[H-pyrrolo{2,3-c}pyridin-2-ylmethyl)-3-pyrrolidinyl}- (9CI) (CA INDEX NAME)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS On STN (Continued)

251938-02-0 CAPLUS
[2,2'-Bithiophene]-5-sulfonamide, 5'-chloro-N-{(3S)-2-oxo-1-{1H-pyrrolo[2,3-c]pyridin-2-ylmethyl}-3-pyrrolidinyl}- {9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251938-03-1 CAPLUS
CN Benzenesulfonamide,
4-(1,1-dimethylethyl)-N-((3S)-2-oxo-1-(1H-pyrrolo(2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251938-04-2 CAPLUS
Thieno[3,2-c]pyridine-2-sulfonamide, 4-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251938-07-5 CAPLUS
Thieno[2,3-c]pyridine-2-sulfonamide, 7-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

251938-08-6 CAPLUS
1H-Benzimidazole-2-sulfonamide, 5-chloro-N-{(3S)-2-oxo-1-(1H-pyrrolo{2,3-clpyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

Cl

IТ 251936-17-1 287203-90-1

Absolute stereochemistry.

287203-90-1 CAPLUS

1H-Pyrrolo[2,3-c]pyridine-1-carboxylic acid, 2-{[(3S)-3-amino-2-oxo-1-pyrrolidinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS On STN
ACCESSION NUMBER: 1999:819359 CAPLUS
DOCUMENT NUMBER: 132:64065
TITLE: Preparation of fluorobenzoylated resins as solid
phase

synthesis supports
Salvino, Joseph M.; Groneberg, Robert D.; Airey, John E.; Poli, Gregory B.; McGeehan, Gerard M.;
Labaudiniere, Richard F.; Clerc, Francois-frederic;
Bezard, Daniel Noel Andre
Rhone-Poullenc Rozer Pharmaceuticals Inc., USA
PCT Int. Appl., 113 pp.
CODEN: PIXXDD
Patent
English
8 INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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		RO,	RU,	SĐ,	SE,	SG,	SI,	SK,	SL,	TJ.	, TM,	TR,	TT.	UA,	UG,	US.	UZ.
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	RW:	GH,	GM,	KΕ,	LS,	MW,	SD,	SL,	SZ,	UG.	, 2W,	AT,	BE,	CH,	CY,	DE,	DK,
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PRIORITY	APP	LN.	INFO	. :						US :	1998-	9055	8P		P 1	9980	624
											1000						

OTHER SOURCE(S): CASREACT 132:64065

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 19 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

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ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) Title resins [I; R = resin; R1-R3 \sim H or ring system substituent (sic);
               = F, OH, alkanoyl- or aroyloxy, SO3H, etc.; Z = 21SO2, Z1NHSO2, Z1CH2CO, Z1Z2, etc.; Z1 = bond, (un)substituted phenylene, -alkylene, etc.; Z2 = (un)substituted phenylene) were prepared The F atom ortho to the loading site permits the absolute loading of the resin to be determined using UNPR
site permits the absolute loading of t

19F NNR.

IT 209285-75-6P 209285-82-5P 209285-84-7P

251936-19-3P 251937-85-6P 251937-86-7P

251937-87-8P 251937-88-9P 251937-99-0P

251937-93-6P 251937-91-4P 251937-95-8P

251937-93-6P 251937-97-0P 251937-98-1P

251937-93-6P 251938-00-8P 251938-04-2P

251938-03-0P 251938-03-1P 251938-04-2P

251938-05-3P 251938-06-4P 251938-07-5P

251938-06-6P

RL SPM (Synthetic preparation); PREP
Absolute stereochemistry.
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RN 209285-82-5 CAPLUS
CN Benzo(b)thiophene-2-sulfonamide,
6-chloro-N-(133)-2-cov-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

209285-84-7 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, N-{(3S)-2-oxo-1-(1H-pyrrolo[2,3-c)pyridin-2-y|methyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251936-19-3 CAPLUS
[2,2'-Bithiophene]-5-sulfonamide, 5'-chloro-N-{(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA IN (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251937-88-9 CAPLUS
Thieno[2,3-b]pyridine-2-sulfonamide, N-{(3S)-2-oxo-1-(1H-pyrrolo[3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl}- (9CI) (CA INDEX NAME)

251937-89-0 CAPLUS 2-Thiophenesulfonamide, 5-(3-iBoxazoly1)-N-[(35)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethy1)-3-pyrrolidiny1]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & &$$

251937-85-6 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, N-[(35)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251937-86-7 CAPLUS
2-Thiophenesulfonamide, N-{(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl}-5-(2-pyridinyl)- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

251937-87-8 CAPLUS Thieno[3,2-b]pyridine-2-sulfonamide, 5-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251937-90-3 CAPLUS
Thieno[2,3-b]pyridine-2-sulfonamide, 6-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251937-91-4 CAPLUS.
CN Benzenesulfonamide,
4-(1,1-dimethylethyl)-N-((35)-2-oxo-1-(1H-pyrrolo(3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251937-92-5 CAPLUS
Thieno[3,2-c)pyridine-2-sulfonamide, 4-chloro-N-{(3S)-2-oxo-1-(1H-pyrroloi3,2-c)pyridin-2-ylmethyl)-3-pyrroloidinyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 251937-93-6 CAPLUS
CN 2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251937-94-7 CAPLUS
CN Benzo[b]thiophene-2-sulfonamide, 5-chloro-3-methyl-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 251937-97-0 CAPLUS
CN 2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251937-98-1 CAPLUS
CN Thieno[3,2-b]pyridine-2-sulfonamide, 5-chloro-N-[(3S)-2-oxo-1-[1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 251937-95-8 CAPLUS
Thieno[2,3-c]pyridine-2-sulfonamide, 7-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251937-96-9 CAPLUS
CN H-Benzimidazole-2-sulfonamide, 5-chloro-N-[(35)-2-oxo-1-(1H-pyrrolo[3,2-cl)pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry

L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 251937-99-2 CAPLUS
CN Thienc(2,3-b)pyridine-2-sulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-y]methyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251938-00-8 CAPLUS
CN 2-Thiophenesulfonamide, 5-(3-isoxazoly1)-N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethy1)-3-pyrrolidiny1]- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 251938-01-9 CAPLUS

Thieno(2,3-b)pyr:dine-2-sulfonamide, 6-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo(2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251938-02-0 CAPLUS (2.2"-Bithiophenel-5-sulfonamide, 5'-chloro-N-((35)-2-oxo-1-(1H-pyrroloi2,3-c]pyridin-2-ylmethyl)-3-pyrroloidinyl)- (9C1) (CA INDEX NAME)

RN 251938-03-1 CAPLUS
CN Benzenesulfonamide,
4-(1,1-dimethylethyl)-N-((3S)-2-oxo-1-(1H-pyrrolo(2,3c)pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251938-04-2 CAPLUS
Thieno[3,2-c]pyridine-2-sulfonamide, 4-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo(2,3-c]pyridin-2-ylmethyl)-3-pyrrolodinyl]- (9CI) (CA INDEX NAME)

ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251938-07-5 CAPLUS
Thieno[2,3-c]pyridine-2-sulfonamide, 7-chloro-N-{(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

251938-08-6 CAPLUS
1H-Benzimidazole-2-sulfonamide, 5-chloro-N-{(35)-2-oxo-1-(1H-pyrrolo{2,3-clpyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251938-05-3 CAPLUS
2-Thiophenesulfonamide, N-{(3S)-2-oxo-1-(1H-pyrrolo{2,3-c}pyridin-2-ylmethyl)-3-pyrrolidinyl}-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

251938-06-4 CAPLUS
Benzo [b] thiophene-2-sulfonamide, 5-chloro-3-methyl-N-[(35)-2-oxo-1-(1H-pyrrolof2,3-c]pyriddin-2-ylmethyl)-3-pyrrolidinyl]- (9Cl) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L6 ANSMER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:784099 CAPLUS
DOCUMENT NUMBER: 132:22881
Sulfonic acid or sulfonylamino N(heteroaralkyl)azaheterocyclic amides as inhibitors

factor Xa
Choi-Sledeski, Yong Mi; Pauls, Heinz W.; Barton,
Jeffrey N.; Ewing, William R.; Green, Daniel M.;
Becker, Michael R.; Gong, Yong; Levell, Julian
Rhone-Poulenc Rorer Pharmaceuticals Inc., USA
CT Int. Appl., 202 pp.
CODEN: PIXXD2
Patent INVENTOR(S):

PATENT ASSIGNEE(S):

DOCUMENT TYPE English LANGUAGE

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATEN	T NO.	ĸ	ND	DATE	:		APPL	I CAT	ION	NO.		r	DATE	
WO 99	62904	,	.1	1999	1209		WO 1	999-	US12	312		• ;	9990	603
W	: AL, AM,	AT, A	, AZ	, BA,	BB,	BG.	BR.	BY.	CA.	CN.	CU.	CZ.	DE.	DK
	EE, ES,	FI, G	, GE	, GH,	Hυ,	IL,	IS,	JP,	KE,	KG.	KP.	KR.	KZ.	LC.
	LK, LR,	LS, L	, LU	, LV,	MD,	MG,	MK,	MN,	MW,	MX.	NO.	NZ.	PL.	PT.
	RO, RU,	SD, SI	, SG	, SI,	sĸ,	SL,	TJ,	TM,	TR,	TT.	UA.	UG.	US.	UZ.
	VN, YU,	ZW, Al	, A2	, BY,	KG,	KZ,	MD,	RU,	TJ.	TM				
R	W: GH, GM,	KE, LS	, MW	, SD,	SL,	SZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,	DK.
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	CI, CM, 02864 33994 43298	GA, G	, GW	, ML,	MR,	NE,	SN,	TD,	TG					
US 66	02864	I	1	2003	0805		U\$ 1:	998-	9049	2		1	9980	603
CA 23	33994		A	1999	1209		CA 1:	999-	2333	994		1	9990	603
AU 99	43298	7	.1	1999	1220		AU 1:	999-	4329	8		1	9990	603
AU 75	8642	1	2	2003	0327									
EP 10	86099	7	.1	2001	0328		EP 1:	999-	9552	66		1	9990	603
R	: AT, BE,	CH, DE	, DK	, ES,	FR,	ĢΒ,	GR,	ĬΤ,	LI,	LU,	NL,	SE,	PT,	ΙE,
	SI, FI 10899 02517393													
BR 99	10899		_	2001	1009		BR 1	999-	1089	9		1	9990	603
JP 20	02517393	1	2	2002	0618		JP 21	000-	5521	15		1	9990	603
VS 62	81227		1	2001	0828		US 1	999-	4533	07		1	9991	202
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JP 20 US 62 NO 20 US 20 PRIORITY A	PPLN. INFU	. :					US 19	998-	9049	2	,	A2 1	9980	603
						1	US 19	996-	3315	9 P	1	P 1	9961	213
						1	WO 19	997-	US22	406	,	A2 1	9971	203
						1	WO 19	999-	US12:	312		1	9990	603
						1	US 19	999-	4533	07	,	A3 1	9991	202

OTHER SOURCE(S): MARPAT 132:22881

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CRN 209286-50-0 CMF C13 H16 N4 O

Absolute stereochemistry

CM

209286-82-8 CAPLUS Carbamic acid, [(3S)-1-[(4-chloro-1-(phenylsulfonyl)-1H-pyrrolo[3,2-c)pyridin-2-yl)methyl]-2-oxo-3-pyrrolidinyl]-, 1,1-dimethylethyl est (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 209286-83-9 CAPLUS
CN 1H-Pyrrolo(3,2-c|pyridine,
2-[[(3S)-3-amino-2-oxo-1-pyrrolidinyl]methyl]-4chloro-1-(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Aza heterocycles I [X = (CHR3)m; R = (un) substituted heteroaryl; R1, R2 = H, (un) substituted alkyl, alkenyl, aralkyl; R3 = H, OH, (un) substituted alkyl, aryl, heteroaryl; R4 = H, (un) substituted alkyl, aryl, aralkyl;

R6 = H; R5R6 = O; R7, R8 = H, (un)substituted alkyl, aryl, aralkyl; heteroaryl; R7R8 = O; R3R7 = alkylene; m = O-3] were prepared I are inhibitors of the activity of Factor Xa. Thus, the amide II was prepared from 3-acctamido-4-methylbenzaldehyde, malonic acid, and 7-methoxy-2-naphthalenesulfonyl chloride in 10 steps. II had a Ki of 80 nm for inhibition of factor Xa.

209286-49-79 209286-51-1P 209286-82-8P 209286-83-99 209286-63-99 209286-81-92 51936-18-2P 251936-22-8P

EXECUTE: A Comparison of the Comparation of the Com

209286-49-7 CAPLUS
Carbamic acid, [(3S)-2-oxo-1-[2-[1H-pyrrolo[3,2-c]pyridin-1-yl]ethyl]-3-pyrrolidinyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

209286-51-1 CAPLUS 2-Pyrrolidinone, 3-amino-1-[2-(1H-pyrrolo[3,2-c]pyridin-1-yl)ethyl]-, (38)-, monoacetate (9CI) (CA INDEX NAME)

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

• HCl

209286-84-0 CAPLUS
Benzo[b] thiophene-2-sulfonamide, 6-chloro-N-[[35]-1-[[4-chloro-1-(phenylsulfonyl)-1H-pyrrolo[3,2-c]pyridin-2-yl]methyl]-2-oxo-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

209287-05-8 CAPLUS
1H-Pyrrolo[2,3-c]pyridine-1-carboxylic acid, 2-[[(3s)-3-[[(6-chorobenzo(b)thien-2-y1)sulfonyl]amino]-2-oxo-1-pyrrolidinyl]methyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251936-16-0 CAPLUS
1H-Pyrrolo[3,2-c]pyridine-1-carboxylic acid, 2-[[(35)-2-oxo-3-[((phenylmethoxy)carbonyl]amino)-1-pyrrolidinyl]methyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251936-17-1 CAPLUS

1H-Pyrrolo[3,2-c]pyridine-1-carboxylic acid, 2-[{(35)-3-amino-2-oxo-1-pyrrolidinyl]methyll-, 1,1-dimethylethyl ester [90]) (CA INDEX NAME)

Absolute stereochemistry.

251936-18-2 CAPLUS

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN INDEX NAME)

СМ 1

209285-46-1 C24 H24 N4 O4 S

Absolute stereochemistry

2

76-05-1 C2 H F3 O2

RN 209285-74-5 CAPLUS
CN Benzo[b]thiophene-2-sulfonamide, 6-chloro-N-[(3S)-1-[(4-chloro-1H-pyrrolo[3,2-c]pyridin-2-y1)methyl)-2-oxo-1-pyrrolidinyl]- (9CI) (CA NAME)

Absolute stereochemistry.

L6 ANSMER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued IN-Pyrrolo[3,2-c]pyridine-1-carboxylic acid, 2-[[[35]-3-[[[5]-chloro[2,2]-bithiophen]-5-pl]sulfonyl]amino]-2-oxo-1-pyrrolidinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251936-22-8 CAPLUS
HH-Pyrrolo[3,2-c]pyridine-1-carboxylic acid, 2-{[[35]-3-[[2-(5-chloro-2-thienyl)=thenyl]=ulfonyl]amino]-2-oxo-1-pyrrolidinyl]methyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

IT

209285-47-2 CAPLUS

2-Naphthalenesulfonamide, 7-methoxy-N-{(3S)-2-oxo-1-[2-(1H-pyrrolo[3,2-c]pyridin-1-yl)ethyl}-3-pyrrolidinyl}-, mono(trifluoroacetate) (9CI) (CA

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

209285-75-6 CAPLUS
Benzo[b]thiophene-2-sulfonamide,
loro-N-[38:3-2-oxo-1-(1H-pyrrolo[3,2c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

bsolute stereochemistry.

RN 209285-82-5 CAPLUS
CN Benzo[b]thiophene-2-sulfonamide,
6-chloro-N-[135]-2-oxo-1-(1R-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 209285-83-6 CAPLUS
CN Benzo(b)thiophene-2-sulfonamide,
6-chloro-N-(38)-2-cxoc-1-(1H-pyrrolo[2,3c)pyridin-2-ylmethyl)-3-pyrrolidinyl)-, mono(trifluoroacetate) (9CI) (CA
INDEX NAME)

CRN 209285-82-5 CMF C20 H17 C1 N4 O3 S2

Absolute stereochemistry.

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

2 CM

76-05-1 C2 H F3 O2

251936-19-3 CAPLUS [2,2'-Bithiophene]-5-sulfonamide, 5'-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251936-23-9 CAPLUS
CN Ethenesulfonamide,
2-(5-chloro-2-thienyl)-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN CRN 76-05-1 CMF C2 H F3 O2

209285-84-7 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

209285-85-8 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209285-84-7 CMF C19 H17 N5 O3 S2

Absolute stereochemistry.

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

251937-85-6 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- [9CI) (CA INDEX NAME)

251937-86-7 CAPLUS
2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251937-87-8 CAPLUS
Thieno[3,2-b]pyridine-2-sulfonamide, 5-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrroloidinyl}- (9CI) (CA INDEX NAME)

L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 251937-88-9 CAPLUS
CN Thieno(2,3-b)pyridine-2-sulfonamide, N-{(35)-2-oxo-1-(1H-pyrrolo(3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251937-89-0 CAPLUS
CN 2-Thiophenesulfonamide, 5-(3-isoxazolyl)-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c)pyridin-2-yimethyl)-3-pyrrolidinyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued Absolute stereochemistry.

RN 251937-93-6 CAPLUS
CN 2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo(3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251937-94-7 CAPLUS
CN Benzo[b]thiophene-2-sulfonamide, 5-chloro-3-methyl-N-{(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 251937-90-3 CAPLUS
CN Thieno[2,3-b]pyridine-2-sulfonamide, 6-chloro-N-[(35)-2-oxo-1-(1H-pyrrolof),2-clpyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)
Absolute stereochemistry.

NH NH O

RN 251937-91-4 CAPLUS
CN Benzenesulfonamide,
4-(1,1-dimethylethyl)-N-{(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251937-92-5 CAPLUS
CN Thieno[3,2-c]pyridine-2-sulfonamide, 4-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo]3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9Cl) (CA INDEX NAME)

L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 251937-95-8 CAPLUS
CN Thieno[2,3-c]pyridine-2-sulfonamide, 7-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251937-96-9 CAPLUS
CN 1H-Benzimidazole-2-sulfonamide, 5-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c)pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 251937-97-0 CAPLUS
CN 2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 251937-98-1 CAPLUS
CN Thieno[3,2-b]pyridine-2-sulfonamide, 5-chloro-N-[{3S}-2-oxo-1-[1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 251938-01-9 CAPLUS
CN Thieno(2,3-b)pyridine-2-sulfonamide, 6-chloro-N-[(3S)-2-oxo-1-(1Hpyrrolo(2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251938-02-0 CAPLUS CN (2,2'-Bithiophene)-5-sulfonamide, 5'-chloro-N-[(3S)-2-oxo-1-(1Hpyrrolo(2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251938-03-1 CAPLUS
CN Benzenesulfonamide,
4-(1,1-dimethylethyl)-N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Con

RN 251937-99-2 CAPLUS
CN Thieno[2,3-b]pyridine-2-sulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251938-00-8 CAPLUS
CN 2-Thiophenesulfonamide, 5-(3-isoxazoly1)-N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-clpyridin-2-ylmethyl)-3-pyrrolidinyl]- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (C

(Continued)

RN 251938-04-2 CAPLUS
CN Thieno(3,2-c)pyridine-2-sulfonamide, 4-chloro-N-{(3S)-2-oxo-1-(1H-pyrrolo[2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251938-05-3 CAPLUS CN 2-Thiophenesulfonamide, N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl)-5-(4-pyridinyl)- (9C1) (CA INDEX NAME)

Absolute stereochemistry

RN 251938-06-4 CAPLUS

Renzo(b)thiophene-2-sulfonamide, 5-chloro-3-methyl-N-[(35)-2-oxo-1-(1H-pyrrolo)(2,3-clpyridin-2-ylmethyl)-3-pyrrolidinyl]- (9C1) (CA INDEX NAME)

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251938-07-5 CAPLUS
Thieno[2,3-c]pyridine-2-sulfonamide, 7-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251938-08-6 CAPLUS
1H-Benzimidazole-2-sulfonamide, 5-chloro-N-[(35)-2-oxo-1-(1H-pyrrolo[2,3-c]pyridin-2-ylmethyl)-3-pyrrolidinyll- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) 251938-39-3 CAPLUS (Glycine, N-[[2-(5-chloro-2-thienyl)ethenyl)sulfonyl]-N-[(3R)-2-oxo-1-(1H-pyrrolo]3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

251938-46-2 CAPLUS Thieno[3,2-b]pyridine-2-sulfonamide, N-[{3R}-2-oxo-1-(1H-pyrrolo[2,3-c)pyridin-2-ylmethyl)-3-pyrrolidinyl]-, bis(trifluoroacetate) (9CI) {CA INDEX NAME}

CM 1

CRN 251938-45-1 CMF C19 H17 N5 O3 S2

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 02

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

251938-35-9 CAPLUS
2-Pyrrolidinone, 1-{(4-amino-7-quinazolinyl)methyl}-3-{(1H-pyrrolo{2,3-c}pyridin-2-ylmethyl)amino}-, (3S)- (9CI) (CA INDEX NAME)

251938-38-2 CAPLUS Ethenesulfonamide, 5-chloro-2-thienyl]-N-[(3R)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L6 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS ON STN

ACCESSION NUMBER: 1998:402310 CAPLUS

DOCUMENT NUMBER: 129:81744

Preparation of sulfonic acid or sulfonylamino N-(heteroaralkyl)-azabeterocyclylamide compounds as inhibitors of factor Xa choi-Sledeski, Yong Mi; Paule, Henry W.; Barton, Jeffrey N.; Ewing, William R.; Green, Daniel M.; Becker, Michael R.; et al.

PATENT ASSIGNEE(S): Rhome-Poulenc Rover Pharmaceuticals Inc., USA PCT Int. Appl., 116 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4 FAMILY ACC. NUM. COUNT:

PATEN	T:	NFOR	MATI	ON:															
	PAT	TENT	NO.			KIN	D	DATE			API	PLI	CAT	ION	NO.		D	ATE	
		9825	611			A1		1998	0618		WO	19	97-1	U\$22	406		1	9971	203
		W:	AL,	AM,	AT,	AU,	AZ,	EA,	BB,	BG,	BI	R,	BY,	CA,	CN,	CU,	CZ.	DE.	DK.
			EE,	ES,	FI,	GB,	GE,	GH,	HU,	IL,	IS	S,	JP,	KE,	KG,	KP,	KR,	KZ.	LC.
			LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MI	κ,	MN,	MW.	MX.	NO.	NZ.	PL.	PT.
			RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	Tá	J,	TM,	TR,	TT.	UA,	UG.	US.	UZ.
			VN,	YU,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MI	٥,	RU,	TJ,	TM				
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	ΑU	7266	37			₿2		2000	1116										
	EΡ	9443	86			A1		1999	0929		ΕP	19	97-	9515	73		1	9971	203
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		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GI	٦,	IT,	LI,	LU,	NL,	SE,	MC.	PT.
			ΙE,	SI,	FI,	RO													
	CN	1244	798			A		2000	0216		CN	19	97-	1813	8,7		1	9971	203
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	JΡ	9713 2001 1032	5066	30		T2		2001	0522		JP	15	98-	5268	44		1	9971	203
	ΑP	1032				A		2001	1224		AΡ	19	99-	1552			1	9971	203.
		W :	GH,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW									
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	ES	2184	145			T3		2003	0401		ES	19	97-	9515	73		1	9971	203
	ZA	9711	207			A		1998	0720		ZA	19	97-	1120	7		1	9971	212
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	KR	2000	0575	28		Α		2000	0925		KR	19	99-	7052	36		1	9990	611
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1	US	2002	0133	10		A1		2002	0131		US	20	01-9	9180	39		2	0010	730
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L6 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) etc.: one of X5, X5a, and X5a - H, H0 or (H, optionally substituted lower alkyl, hydroxy, alkoxy, or aminolNH that substitutes the distal ring of Arl at a position alpha to a nitrogen thereof) herein exhibit useful pharmacol. activity and accordingly are incorporated into pharmaceutical compns. and used in the treatment of patients suffering from certain medical disorders. More specifically, they are inhibitors of the activity of Factor Xa. The present invention is directed to compds. of formula I, compns. contg. compds. of formula I, and their use, which are for treating a patient suffering from, or subject to, physiol. condition (disorder) which can be ameliorated by the administration of an inhibitor of the activity of Factor Xa. The physiol disorder is venous vasculature, arterial vanculature, abnormal thrombus formation, acute myocardial infarction, unstable angina, thromboembolism, acute vessel closure assocd.

with thrombolytic therapy, percutaneous transluminal coronary

angioplasty, transient ischemic attacks, stroke, intermittent claudication or bypass grafting of the coronary or peripheral arteries, vessel luminal

grafting of the coronary or peripheral access, which are made of the coronary or venous angioplasty, maintenance of vascular access patency in long-term hendialysis patients, pathol. thrombus formation occurring in the veins of the lower extremities following abdominal, knee and hip surgery, a risk of pulmonary thromboembolism, or disseminated systemic intravascular coagulopathy occurring in vascular systems during septic shock, certain viral infections and cancer. Thus, 3-(S)-amino-1-(6-amino-1-chloroisoquinolin-7-ylmethyl)pyrrolidin-2-one

coupled with 7-methoxynaphthalene-2-sulfonyl chloride followed by amination with ammonium acetate in PhOH at 115° for 2 h gave the

amination with ammonium acetate in PhOH at 115° for 2 h gave the title compd.

N-[N-(isoquinolinylmethyl)oxopyrrolidinyl]naphthalenesulfona mide (II.CF3CO2H). II.CF3CO2H in vitro inhibited factor Xa, thrombin, trypsin, tissue-plasminogen activator (t-PA), plasmin and activated protein C with Ki value of 80 nM.

IT 209285-47-2P 209285-74-5P 209285-75-6P
209285-83-6P 209285-88-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

logical study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of sulfonic acid or sulfonylamino N-(heteroaralkyl)-azaheterocyclylamide compds. as inhibitors of factor Xa) 209285-47-2 CAPLUS

2-Naphthalenesulfonnmide, 7-methoxy-N-[(3S)-2-oxo-1-[2-(1H-pyrrolo[3,2-c]pyridin-1-yl]ethyl]-3-pyrrolidinyl]-, mono(trifluoroacetate) (9CI) NIDEX NAME

CM 1

CRN 209285-46-1 CMF C24 H24 N4 O4 S

Absolute stereochemistry.

L6 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN WO 1999-US12312 A2 19990603

> US 1999-453307 A3 19991202

OTHER SOURCE(S):

MARPAT 129:81744

AB The compds of formula [I; Arl = a bicyclic heteroaryl containing ≥ 1 N atom; Z = alkenyl; R1 = H, (un)substituted alkyl, aralkyl, or heteroalkyl, hydroxyalkyl, carboxy alkyl, carbamoylalkyl, aminoalkyl, etc.; R2 = R3S(O)p, R384NS(O)p; R3 = (un)substituted alkyl, cycloalkyl, heterocyclyl,

RASIGUP, RASEABLOTP; RS = LANTAUSSECTIONS AND ASSECTIONS AND ASSECTION ASSEC

X3 = H, OH, (un)substituted alkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl; or X3 or one of X1 and X1a taken together form a 4 to 7 membered cycloalkyl; X5, X5a, X5b = H, (un)substituted NH2, HONH, alkoxyamino, NHNH2, (un)substituted OH. CONH2 or SOZNH2, halo, cyano,

ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 209285-74-5 CAPLUS
CN Benzo[b]thiophene-2-sulfonamide, 6-chloro-N-{(3S)-1-[(4-chloro-H-pyrrolo[3,2-c]pyridin-2-yl)methyl]-2-oxo-3-pyrrolidinyl]- (9CI) (
INDEX

Absolute stereochemistry.

RN 209285-75-6 CAPLUS
CN Benzo[b]thiophene-2-sulfonamide,
6-chloro-N-[(3S)-2-oxo-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 209285-83-6 CAPLUS
CN Benzo(b)thiophene-2-sulfonamide,
6-chloro-N-[435]-2-cxc-1-[1H-pyrrolo[2,3clpyridin-2-ylmethyl]-3-pyrrolidinyl]-, mono(trifluoroacetate) [9CI] (CA
INDEX NAME)

CRN 209285-82-5 CMF C20 H17 C1 N4 O3 S2

Absolute stereochemistry.

ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IT

209286-49-7P 209286-51-1P 209286-82-8P
209286-83-9P 209286-84-0P 209287-05-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfonic acid or sulfonylamino N-(heteroaralkyl)-azaheterocyclylamide compds. as inhibitors of factor Xa)
209286-49-7 CAPLUS
Carbamic acid, [(3S)-2-0xo-1-[2-(1H-pyrrolo[3,2-c]pyridin-1-yl)ethyl]-3-pyrrolidinyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

209286-51-1 CAPLUS
2-Pyrrolidinone, 3-amino-1-[2-(1H-pyrrolo[3,2-c]pyridin-1-y1)ethyl]-,
(3S)-, monacetate [9CI) (CA INDEX NAME)

CM 1

CRN 209286-50-0 CMF C13 H16 N4 O

Absolute stereochemistry.

2

209286-82-8 CAPLUS Carbamic acid, {(35)-1-{(4-chloro-1-(phenylsulfonyl)-1H-pyrrolo(3,2-c)pyridin-2-yl]methyl]-2-oxo-3-pyrrolidinyl]-, 1,1-dimethylethyl ester (9C1) (CA INDEX NAME)

Absolute stereochemistry.

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN CRN 76-05-1 CMF C2 H F3 O2 (Continued)

209285-85-8 CAPLUS Thieno(3,2-b]pyridine-2-sulfonamide, N-[(35)-2-oxo-1-(1H-pyrrolo(2,3-c)pyridin-2-yhmethyl)-3-pyrrolidinyl}-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 209285-84-7 CMF C19 H17 N5 O3 S2

Absolute stereochemistry.

ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 209286-83-9 CAPLUS
CN 1H-Pyrrolo(3,2-c]pyridine,
2-[(3S)-3-mino-2-oxo-1-pyrrolidinyl]methyl]-4chloro-1-(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

• HCl

209286-84-0 CAPLUS
Benzo[b]thiophene-2-sulfonamide, 6-chloro-N-[(3S)-1-[(4-chloro-1-(phenylsulfonyl)-1H-pyrrolo(3,2-c]pyridin-2-yl]methyl]-2-oxo-3-pyrrolidinyl]- (9Cl) (CA INDEX NAME)

L6 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 209287-05-8 CAPLUS
CN 1H-Pyrrolo(2,3-c]pyridine-1-carboxylic acid, 2-[[(3S)-3-[[(6-chlorobenzo(b] thien-2-yl) sulfonyl]amino]-2-oxo-1-pyrrolidinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THE

FORMAT

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=> s 15 and (factor xa or diagnos? or cardioprotect? or direct thrombin inhibit? or
anticoaqula? or antiplatelet or fibrinoloyt? or heparin or fibrinoqen or
streptokinase or urokinase or tissue plasminogen activator or tpa)
            10 L5
        902352 FACTOR
        804002 FACTORS
       1424586 FACTOR
                  (FACTOR OR FACTORS)
          8728 XA
         13639 XAS
         22358 XA
                  (XA OR XAS)
          5468 FACTOR XA
                  (FACTOR (W) XA)
        231283 DIAGNOS?
          7907 CARDIOPROTECT?
        568995 DIRECT
          7067 DIRECTS
        575210 DIRECT
                  (DIRECT OR DIRECTS)
         33287 THROMBIN
           193 THROMBINS
         33292 THROMBIN
                  (THROMBIN OR THROMBINS)
       1750384 INHIBIT?
           516 DIRECT THROMBIN INHIBIT?
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          4256 ANTIPLATELET
            56 ANTIPLATELETS
          4281 ANTIPLATELET
                  (ANTIPLATELET OR ANTIPLATELETS)
             1 FIBRINOLOYT?
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          1716 HEPARINS
         45437 HEPARIN
                  (HEPARIN OR HEPARINS)
         28619 FIBRINOGEN
         15455 FIBRINOGENS
         30871 FIBRINOGEN
                  (FIBRINOGEN OR FIBRINOGENS)
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        641280 TISSUE
        315311 TISSUES
        818920 TISSUE
                  (TISSUE OR TISSUES)
         26300 PLASMINOGEN
           174 PLASMINOGENS
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(PLASMINOGEN OR PLASMINOGENS)

26310 PLASMINOGEN

43 TPAS

17233 TPA

(TPA OR TPAS)

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9 L5 AND (FACTOR XA OR DIAGNOS? OR CARDIOPROTECT? OR DIRECT THROMB IN INHIBIT? OR ANTICOAGULA? OR ANTIPLATELET OR FIBRINOLOYT? OR HEPARIN OR FIBRINOGEN OR STREPTOKINASE OR UROKINASE OR TISSUE PLASMINOGEN ACTIVATOR OR TPA)

=> s 1-9 ibib abs 8307201 1 1757794 9 14 IBIB 220746 ABS L8 0 1-9 IBIB ABS (1(W)9(W)IBIB(W)ABS)

=> del 18 y;d 1-9 ibib abs

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 2004:832890 CAPLUS DOCUMENT NUMBER: 142:19473 142:19473
Comparing Ligand Interactions with Multiple Receptors via Serial Docking
Fernandes, Miguel X.; Kairys, Visvaldas; Gilson, Michael K.
Center for Advanced Research in Biotechnology, U.
Maryland Biotechnology Institute, Rockville, MD, 20850, USA
Journal of Chemical Information and Computer Sciences (2004), 44(6), 1961-1970
CODEN; JCISDB; ISSN: 0095-2338
American Chemical Society
Journal TITLE: AUTHOR(S): CORPORATE SOURCE: SOURCE: PUBLISHER: DOCUMENT TYPE: LANGUAGE: Journal JAGE: English
Standard uses of ligand-receptor docking typically focus on the AB Standard uses of a sassociation of candidate ligands with a single targeted receptor, but actual cations increasingly require comparisons across multiple receptors. This study demonstrates that comparative docking to multiple receptors can help to select homol. models for virtual compound screening and to discover that bind to one set of receptors but not to another, potentially ar, set. A serial docking algorithm is furthermore described that reduces computational costs of such calens, by testing compds, against a series receptor structures and discarding a compound as soon as it fails to satisfy
specified bind/no bind criteria for each receptor. The algorithm also
realizes substantial efficiencies by taking advantage of the fact that a
ligand typically binds in similar conformations to similar receptors.
Thus, once detailed docking has been used to fit a ligand into the first
of a series of similar receptors, much less extensive calons, can be used
for the remaining structures.

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:894400 CAPLUS
DOCUMENT NUMBER: 138:133092
TITLE: Crystal Structures of Two Potent Nonamidine
Inhibitors TITLE: Crystal Structures of Two Potent Nonamidine Inhibitors

Bound to Factor IA

AUTHOR(S): Adler, Marc; Kochanny, Monica J.; Ye, Bin; Rumennik, Galina; Light, David R.; Biancalana, Sara; Whitlow, Marc

CORPORATE SOURCE: Berlex Biosciences, Richmond, CA, 94804-0099, USA
Biochemistry (2002), 41(52), 15514-15523

CODEN: BICHAW; ISSN: 0006-2960

American Chemical Society

Journal
LANGUAGE: American Chemical Society

Journal
LANGUAGE: There has been intense interest in the development of factor

IA inhibitors for the treatment of thrombotic diseases. Our laboratory has developed a series of novel non-amidine inhibitors of factor

IA. This paper presents two crystal atructures of compds. from this series bound to factor IA. The first structure is derived from the complex formed between factor IA and compound 1. Compound 1 was the first non-amidine factor

IA inhibitor from our laboratory that had measurable potency in an in vitro assay of anticosquent activity. The second compound, 2, has a molar affinity for factor IA (Kiapp) of 7 pM and good bioavailability. The two inhibitors bind in an L-shaped conformation

with a chloroarom. ring buried deeply in the S1 pocket. The opposite end conformation
with a chloroarom. ring buried deeply in the S1 pocket. The opposite end
of these compds. contains a basic substituent that extends into the S4
binding site. A chlorinated Ph ring bridges the substituents in the S1
and S4 pockets via amide linkers. The overall conformation is similar to
the previously published structures for amidine-based inhibitors
complexed
with factor Ts. However, there are significant exed with factor Xa. However, there are significant differences in the interactions between the inhibitor and the protein at the atomic level. Most notably, there is no group that forms a salt bridge with the carboxylic acid at the base of the S1 pocket (Asp189). Ea inhibitor forms only one well-defined hydrogen bond to the protein. There
are no direct charge-charge interactions. The results indicate that
electrostatic interactions play a secondary role in the binding of these
potent inhibitors.

REFERENCE COUNT: 30 THERE ARE 30 CITED REPERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2003:89919 CAPLUS DOCUMENT NUMBER: 138:247939 138:247939
Discovery of an orally efficacious inhibitor of coagulation factor Xa which incorporates a neutral Pl ligand Choi-Sledeski, Yong Mi, Kearney, Robert; Poli, Gregory; Paula, Henry; Gardner, Charlee; Gong, Yong; Becker, Michael; Davis, Roderick; Spada, Alfred; Liang, Guyan; Chu, Valeria; Brown, Karen; Collussi, Dennis; Leadley, Robert, Jr.; Rebello, Sam; Moxey, Phillip; Morgan, Suzanne; Bentley, Rose; Kasiewski, Charles; Maignan, Sebastien; Guilloteau, Jean-Pierre; Mikol, Vincent TITLE: AUTHOR(S): Charles; Maignan, Sebastien; Guilloteau, Jean-Pierre; Mikol, Vincent Department of Medicinal Chemistry, Aventis Pharmaceuticals, Bridgewater, NJ, 08807-0800, USA Journal of Medicinal Chemistry (2003), 46(5), 681-684 CODEN: JMCMAR; ISSN: 0022-2623 American Chemical Society Journal CORPORATE SOURCE: SOURCE: PUBLISHER: DOCUMENT TYPE: LANGUAGE: English CASREACT 138:247939 OTHER SOURCE (S):

The discovery and SAR of ketopiperazino methylazaindole factor

In inhibitors are described. Structure-activity data suggesting
that this class of inhibitors does not bind in the canonical mode were
confirmed by an X-ray crystal structure showing the neutral haloarom.
bound in the SI subsite. The most potent azaindole (I, RPR209685), is
selective against related serine protesses and attains higher levels of
exposure upon oral dosing than comparable benzamidines and benzamidine
isosteres. Compound I was efficacious in the canine AV model of
mbosis. 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT:

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

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L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2005 ACS ON STN
ACCESSION NUMBER: 2001:630893 CAPLUS
TITLE: 15:195505

INVENTOR(S): Factor IA inhibitors factor IA inhibitors (Choi-Sledeski, Yong Mi; Pauls, Heinz W.; Barton, Jeffrey N.; Ewing, William R.; Green, Daniel M.; Becker, Michael R.; Gong, Yong: Levell, Julian Aventie Pharma Deutschland GmbH, Germany U.S., 96 pp., Cont.-in-part of U.S. Ser. No. 90,492.
CDCUMENT TYPE: Pathic IA CCL. NUM. COUNT: 4
  DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                  PATENT NO. KIND DATE APPLICATION NO. DATE

105 6281227 B1 20010828 US 1999-453307 19991202 NO 19825611 A1 19986618 NO 1997-US22406 19971203 NO 1997-US22406 NO 1997-US22406 NO 1997-US22406 NO 1997-US22406 NO 1997-US22406 NO 1997-US22406 A2 19971203 
                                                                                                                                                                                                                   KIND
                                                                                                                                                                                                                                                              DATE
                                                                                                                                                                                                                                                                                                                                                                         APPLICATION NO.
    PRIORITY APPLN. INFO .:
                                                                                                                                                                                                                                                                                                                                                                           WO 1997-US22406
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               A2 19971203
                                                                                                                                                                                                                                                                                                                                                                           US 1998-90492
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               A2 19980603
                                                                                                                                                                                                                                                                                                                                                                           WO 1999-US12312
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             A2 19990603
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                                                                                                                                                                                                                                                                                                                                                                           US 1999-453307
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L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN OTHER SOURCE(S): MARPAT 135:195505 (Continued)

Title compds. [I; X = (CHR3)m; R = (un)substituted heteroaryl; R1, R2 =(un)substituted alkyl, alkenyl, aralkyl; R3 = H, OH, (un)substituted alkyl, aryl, heteroaryl; R4 = H, (un)substituted alkyl, aryl, aralkyl;

R6 = H; R5R6 = O; R7, R8 = H, (un)substituted alkyl, aryl, aralkyl, heteroaryl; R7R8 = O; R3R7 = alkylene; m = 0-3] were prepared Thus title

compound II was prepared from 3-acetamido-4-methylbenzaldehyde, malonic acid.

and 7-methoxy-2-naphthalenesulfonyl chloride in 10 steps. II had a Ki of 80 mM for inhibition of **factor IA**.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 5 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
Title compds. {(un)substituted I; R = N-containing heteroaryl; R1 = H,
(acyl)alkyl, (hetero)arylalkyl, etc.; R2 = H, (hetero)arylalkyl,
carbamoylalkyl, etc.; Z = (NH- or NHCO-interrupted or -terminated)
alkylene; Z1 = (CH2)0-3] were prepared Thus, I (R1 = H, Z1 = CH2)(II; R AB

H, R2 = CO2cMe3, Z = bond) was N-alkylated by 7-bromomethyl-1-chloroisoquinoline (preparation each given) and the deprotected product N-acylated by 7-methoxynaphthalene-2-sulfonyl chloride (preparation given) to

give. in 2 addnl. steps, II (R = 1-amino-7-isoquinoly1, R2 = 7-methoxynaphthalene-2-sulfony1, 2 = CH2). Data for biol. activity of I were given

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2001:416755 CAPLUS DOCUMENT NUMBER: 135:46882 TITLE: Prepare:

TITLE: Preparation of N-(oxopyrrolidinyl)naphthalenesulfonami

des and analogs as factor Xa

inhibitors INVENTOR (S):

inhibitors
Choi-Sledeski, Yong Mi; Pauls, Heinz W.; Barton,
Jeffrey N.; Ewing, William R.; Green, Daniel M.;
Becker, Michael R.; Gong, Yong; Levell, Julian
Aventis Pharma Deutschland G.m.b.H., Germany
PCT Int. Appl., 106 pp.
CODEN: PIXXD2

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: Patent English FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE

APPLICATION NO. DATE WO 2001039759 WO 2001039759 A2 A3 20010607 WO 2000-EP11577 20001121 20020117 039759 A3 20020117
AE. AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, II, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, IR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, GH, GM, KE, LS, MN, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG W: AE, AG, CR, CU, HU, ID, US 6281227 PRIORITY APPLN. INFO.: US 1999-453307 A 19991202 US 1996-33159P P 19961213 WO 1997-US22406 A2 19971203 US 1998-90492 A2 19980603

WO 1999-US12312

A2 19990603

OTHER SOURCE(S): MARPAT 135:46082

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 2000:543073 CAPLUS DOCUMENT NUMBER: 133:2610°1 Crystal Structures of Human Factor

In Complexed with Potent Inhibitors
Maignan, Sebastien; Guilloteau, Jean-Pierre; AUTHOR (S) : Pouzieux.

Stephanie; Choi-Sledeski, Yong Mi; Becker, Michael

Klein, Scott I.; Ewing, William R.; Pauls, Henry W.; Spada, Alfred P.; Mikol, Vincent Department of Structural Biology, Aventis Pharma, Vitry/Seine, F-94403, Fr. Journal of Medicinal Chemistry (2000), 43(17), 1236-2232 CODEN: JMCMAR; ISSN: 0022-2623 American Chemical Society

CORPORATE SOURCE:

SOURCE:

3226-2232

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Involved in the coagulation cascade, factor Image: Although there is a great wealth of structural data on thrombin complexes, few structures of ligand/FXs complexes have been reported, presumably because of the difficulty in growing crystals. Reproducible crystallization conditions for human des-Glal-45 coagulation FXs have been found. This has led to an improvement in the diffraction quality of the crystals (about 2.1 Å) when compared to the previously reported forms (2.3-2.8 Å) thus providing a suitable platform for a structure-based drug design approach. A series of crystal structures of moncovalent inhibitors complexed with FXs have been determined, three of which are presented herein. These include

compds. containing the benzamidine moiety and surrogates of the basic

group.

The benzamidine-containing compound binds in a canonical fashion typical

synthetic serine protease inhibitors. On the contrary, mols. that contain

contain

Surrogates of the benzamidine group do not make direct hydrogen-bonding interactions with the carboxylate of Asp189 at the bottom of the S1 pocket. The structural data provide a likely explanation for the specificity of these inhibitors and a great aid in the design of bioavailable potent FXa inhibitors.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSMER 7 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2000:379659 CAPLUS DOCUMENT NUMBER: 133:144473 Solid-phase parallel supplementations. 133:144473
Solid-phase parallel synthesis of azarene pyrrolidinones as factor IX inhibitors
Gong, Yong; Becker, Michael; Choi-Sledeski, Yong Mi; Davis, Roderick S.; Salvino, Joseph M.; Chu, Valeria; Brown, Karen D.; Paule, Henry W.
Department of Medicinal Chemistry, Rhone-Poulenc Rorer, Collegeville, PA, 19426, USA
Bioorganic & Medicinal Chemistry Letters (2000), 10(10), 1033-1036
CDIEN: BMCLES, ISSN: 0960-894X
Elsevier Science Ltd.
Journal English AUTHOR (S): CORPORATE SOURCE: SOURCE: PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): English CASREACT 133:144473

A focused library (4+14) prepared from 4-aminopyridine and 4-, 5-, and 6-azoindole templates was synthesized using 14 polymer-supported 4-amido-2,3-5,6-terfafluorophenyl (TFP) sulfonate esters and heteroarylmethyl-substituted arylsulfonylamino pyrrolidinones such as I

give a library of factor Is inhibitors such as II.

Several compds. were identified as factor Is
inhibitors (ICSOSO.1 MM) helping to establish the SAR among
these four series of azarene pyrrolidinones. E.g., factor
Is was inhibited by II with a Ki of 15 nM
RENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR

REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 8 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

NR1p2

Aza heterocycles I $\{X = (CHR3)m; R = (un)$ substituted heteroaryl; R1, R2 = H, (un)substituted alkyl, alkenyl, aralkyl; R3 = H, OH, (un)substituted alkyl, aryl, heteroaryl; R4 = H, (un) substituted alkyl, aryl, aralkyl;

R6 = H; R5R6 = O; R7, R8 = H, (un)substituted slkyl, aryl, aralkyl, heteroaryl; R7R8 = O; R3R7 = alkylene; m = 0-3] were prepared I are inhibitors of the activity of *Pactor *La. Thus, the amide II was prepared from 3-acetamido-4-methylbenzaldehyde, malonic

acid,
and 7-methoxy-2-naphthalenesulfonyl chloride in 10 steps. II had a Ki of
80 mM for inhibition of factor Xa.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

FORMAT

L7 ANSMER 8 OF 9 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 1999:784099 CAPLUS DOCUMENT NUMBER: 132:22881 TITLE: Sulfons and the state of th ulfonic acid or sulfonylamino N-(heteroaralkyl) azaheterocyclic amides as inhibitors of Choi-Sledeki, Yong Mi; Pauls, Heinz W.; Barton, Jeffrey N.; Ewing, William R.; Green, Daniel M.; Becker, Michael R.; Gong, Yong; Levell, Julian Rhone-Poulenc Rorer Pharmaceuticals Inc., USA PCT Int. Appl., 202 pp.
CODEN: PIXXD2 INVENTOR (S): . PATENT ASSIGNEE(S): DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. 9962904 A1 19991209 M0 1999-US12312 19990603
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MN, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MM, SD, SL, SZ, UG, ZM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI, CM, GA, GM, GM, ML, MR, NE, SN, TD, TG
6602864 B1 20030805 US 1998-90492 19980603
2943298 A1 19991220 A1 1999-2333994 19990603
7958642 B2 20030327 KIND DATE APPLICATION NO. DATE WO 9962904 US 6602864 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI BR 9910899 20011009 BR 1999-10899 19990603 JP 2000-552115 US 1999-453307 NO 2000-5912 JP 2002517393 20020618 19990603 US 6281227 20010828 19991202 NO 2000005912 20010131 20001122 US 2002013310 PRIORITY APPLN. INFO.: 20020131 US 2001-918039 US 1998-90492 A2 19980603 US 1996-33159P P 19961213 WO 1997-US22406 A2 19971203 W 19990603 WO 1999-US12312 US 1999-453307 A3 19991202

L7 ANSWER 9 OF 9 ACCESSION NUMBER: DOCUMENT NUMBER: TITLE:

MARPAT 132:22881

CAPLUS COPYRIGHT 2005 ACS on STN

1998:402310 CAPLUS

129:81744

Preparation of sulfonic acid or sulfonylamino
N-(heteroaralkyl)-azaheterocyclylamide compounds as
inhibitors of factor Xa

Choi-Sledeski, Yong Mi; Pauls, Henry W.; Barton,
Jeffrey N.; Ewing, William R.; Green, Daniel M.;
Becker, Michael R.; et al.
Rhone-Poulenc Rorer Pharmaceuticals Inc., USA
PCT Int. Appl., 116 pp.
CODEN: PIXXD2
Patent
English

NUNT: 4 INVENTOR (S):

PATENT ASSIGNEE (S) : SOURCE:

DOCUMENT TYPE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

OTHER SOURCE(S):

APPLICATION NO. PATENT NO. KIND DATE

WO 1999-US12312

US 1999-453307

A2 19990603

A3 19991202

L7 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2005 ACS On STN OTHER SOURCE(S): MARPAT 129:81744 (Continued)

The compds. of formula [I; Arl = a bicyclic heteroaryl containing ≥ 1 N atom; Z = alkenyl; R1 = H, (un)substituted alkyl, aralkyl, or AB heteroalkyl.

heteroalkyl,
hydroxyalkyl, carboxy alkyl, carbamoylalkyl, aminoalkyl, etc.: R2 =
R35(0)p, R3R4NS(0)p; R3 = (un)substituted alkyl, cycloalkyl,
heterocyclyl,
aryl, heteroaryl, aralkyl, heteroaralkyl, aralkenyl, heteroaralkenyl; or
R1 and R3 taken together with N(0)p or NS(0)pNR4 through which R1 and R3
are linked from a 5 to 7 membered (un)substituted heterocyclyl; wherein p
= 1, 2; R4 = (un)substituted alkyl, cycloalkyl, heteroaryl, etc.; X1, X1a = H, (un)substituted alkyl, aryl, aralkyl,
heteroaryl, etc.; X1, X1a = H, (un)substituted alkyl, aryl, aralkyl,
heteroaryl, or heteroaralkyl; or X and X1a are taken together to form
oxc;

X3 = H, OH, (un)substituted alkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl; or X3 or one of X1 and X1a taken together form a 4 to 7 membered cycloalkyl; X5, X5a, X5b = H, (un)substituted NH2, HONH, alkoxyamino, NHNH2, (un)substituted OH, CONH2 or SOZNH2, halo, cyano,

etc.; one of X5, X5a, and X5a = H, HO or (H, optionally substituted lower alkyl, hydroxy, alkoxy, or amino)NH that substitutes the distal ring of Arı at a position alpha to a nitrogen thereof) herein exhibit useful

ANSWER 9 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) pharmacol. activity and accordingly are incorporated into pharmaceutical compns. and used in the treatment of patients suffering from certain medical disorders. More specifically, they are inhibitors of the

activity

of Factor IA. The present invention is directed to
compds. of formula I, compns. contg. compds. of formula I, and their use,
which are for treating a patient suffering from, or subject to, physiol.
condition (disorder) which can be ameliorated by the administration of an
inhibitor of the activity of Factor IA. The physiol.
disorder is venous vasculature, arterial vasculature, abnormal thrombus
formation, acute myocardial infarction, unstable angina, thromboembolism,
acute vessel closure assocd. with thrombolytic therapy, percutaneous
transluminal coronary angioplasty, transient ischemic attacks, stroke,
intermittent claudication or bypass grafting of the coronary or
peripheral
arteries, vessel luminal narrowing, restenosis post-coronary or venous

arteries, vessel luminal narrowing, restenosis post-coronary or venous angioplasty, maintenance of vascular access patency in long-term hemodialysis patients, pathol. thrombus formation occurring in the veins of the lower extremities following abdominal, knee and hip surgery, a

of pulmonary thromboembolism, or disseminated systemic intravascular coagulopathy occurring in vascular systems during septic shock, certain viral infections and cancer. Thus, 3-(S)-amino-1-(6-amino-1-chloroisequinolin-7-ylmethyllpyrrolidin-2-one was coupled with 7-methoxynaphthalene-2-sulfonyl chloride followed by amination with ammonium acetate in PhOH at 115 for 2 h gave the title compd. N-(N-(isequinolinylmethyl)oxopyrrolidinyl)naphthalenesulfonamide (III.CP3CO2H) II.CP3CO2H in vitro inhibited factor Imalian (III.CP3CO2H), II.CP3CO2H in vitro inhibited factor activator (t-PA), plasmin and activated protein C with Ki value of 80 nM.

80 nM. REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

Prepared by: Mary Hale @2-2507 Rem Bldq 1D86

=> s choi sledeski y?/au pr sledeski y?/au or mi choi sledeski y?/au
'?' TRUNCATION SYMBOL NOT VALID WITHIN 'CHOI SLEDESKI Y?/AU PR SLEDESKI Y?'
The truncation symbol ? may be used only at the end of a search
term. To specify a variable character within a word use '!', e.g.,
'wom!n' to search for both 'woman' and 'women'. Enter "HELP
TRUNCATION" at an arrow prompt (=>) for more information.

=> s choi sledeski y?/au or sledeski y?/au or mi choi sledeski y?/au

30 CHOI SLEDESKI Y?/AU

0 SLEDESKI Y?/AU

0 MI CHOI SLEDESKI Y?/AU

L8 30 CHOI SLEDESKI Y?/AU OR SLEDESKI Y?/AU OR MI CHOI SLEDESKI Y?/AU

=> s ?pyrrolopyridine? and 18

698 ?PYRROLOPYRIDINE?

L9 0 ?PYRROLOPYRIDINE? AND L8

-=> s 18 and 16

L10 7 L8 AND L6

=> d 1-7 ibib abs

L10 ANSWER 1 OF 7
ACCESSION NUMBER:
DOCUMENT NUMBER:
138:247939
Discovery of an orally efficacious inhibitor of coagulation factor Xa which incorporates a neutral P1 ligand
AUTHOR(S):
AUTHOR(S):
CAPLUS COPYRIGHT 2005 ACS on STN
2003:89919 CAPLUS
Discovery of an orally efficacious inhibitor of coagulation factor Xa which incorporates a neutral P1 ligand
Choi-sladeski, Yong M1; Kearney, Robert;
P011, Gregory, Pauls, Henry, Gardner, Charles; Gong, Yong; Becker, Michael; Davis, Roderick; Spada,

SOURCE:

Liang, Guyan; Chu, Valeria; Brown, Karen; Collussi, Dennis; Leadley, Robert, Jr.; Rebello, Sam; Moxey, Phillip; Morgan, Suxanne; Bentley, Ross; Kasiewski, Charles; Maignan, Sebastien; Guilloteau, Jean-Pierre; Mikol, Vincent Department of Medicinal Chemistry, Aventis Pharmaceuticals, Bridgewater, NJ, 08807-0800, USA Journal of Medicinal Chemistry (2003), 46(5), 681-684 CODEN: JMCMAR; ISSN: 0022-3623 American Chemical Society Journal English CASREACT 138:247939

CORPORATE SOURCE:

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

The discovery and SAR of ketopiperazino methylazaindole factor Xa inhibitors are described. Structure-activity data suggesting that this class of inhibitors does not bind in the canonical mode were confirmed by an X-ray crystal structure showing the neutral haloarom. bound in the SI subsite. The most potent azaindole (I, RPR209685) is selective against related serime proteases and attains higher levels of exposure upon oral dosing than comparable benzamidines and benzamidine isosteres. Compound

was efficacious in the camine AV model of thrombosis.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L10 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) WO 1999-US12312 A2 19990603

US 1999-453307 A 19991202

OTHER SOURCE(S):

MARPAT 135:195505

Title compds. [I; X = (CHR3)m; R = (un)substituted heteroaryl; R1, R2 = (un) substituted alkyl, alkenyl, aralkyl; R3 = H, OH, (un) substituted
alkyl, aryl, heteroaryl; R4 = H, (un) substituted alkyl, aryl, aralkyl;

R6 = H; R5R6 = O; R7, R8 = H, (un)substituted alkyl, aryl, aralkyl, heteroaryl; R7R8 = O; R3R7 = alkylene; m = 0-3] were prepared Thus,

compound II was prepared from 3-acetamido-4-methylbenzaldehyde, malonic

acid,
and 7-methoxy-2-naphthalenesulfonyl chloride in 10 steps. II had a Ki of
80 nM for inhibition of factor Xa.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

L10 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 2001:630893 CAPLUS DOCUMENT NUMBER: 135:195505 DOCUMENT NUMBER: TITLE:

INVENTOR(S):

135:195505
Preparation of azaheterocyclic sulfonamides as factor Xa inhibitors
Choi-Sledeski, Yong Mi; Pauls, Heinz W.;
Barton, Jeffrey N.; Ewing, William R.; Green, Daniel M.; Becker, Michael R.; Gong, Yong; Levell, Julian Aventis Pharma Deutschland GmbH, Germany U.S., 96 pp., Cont.-in-part of U.S. Ser. No. 90,492.
CODEN: USXXXAM
Patent PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English

FAIENI INFOR					,						
PATENT I	NO.	K1	ND DA	TE	API	PLICAT	ION NO.				
US 6281:							453307				
WO 9825		Ä					453307 US22406			9912	
W:										9712	
,	EE, ES,	AL, AL	, AZ, B	м, вв,	BG, B	K, BY,	CA, CN	, cu,	CZ,	DE,	DK,
	LK, LR,	F1, G2	, GE, G	n, no,	1L, 13	, JP,	KE, KG	, KP,	KR,	KZ,	rc,
	RO, RU,										
	VN, YU,							, UA,	uu,	US,	υz,
DW.	GH, KE,	TO MI	, A2, D	7 110	710 37	, KU,	13, 1M	D./			
	GB, GR,	IF IT	, 3D, 3	Z, UG,	DT C	, BE,	CH, DE	, DK,	ES,	F1,	FR,
	GN, ML,				F1, 50	., BF,	BJ, Cr	,,	CI,	CM,	ĢΑ,
US 66028		E			US	1008-	90492		19	0000	0.2
WO 9962		P					US12312				
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RW:	GH, GM,							CH.	CY.	DE.	DK.
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WO 20010									20	0011	21
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	LU, LV,	MA, MD	, MG, M	K, MN,	MW, MX	, MZ,	NO, NZ	PL,	PT,	RO,	RU,
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PRIORITY APPI	N. INFO	.:			US	1996-	33159P	1	P 19	9612	13
					wo	1997-1	US22406	2	A2 19	9712	03

L10 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 2001:416755 CAPLUS DOCUMENT NUMBER: 135:46082 TITLE: Preparation of N-(oxopyrrolidinyl)naphthalenesulfonami

naleneaulronami
des and analogs as factor Xa inhibitors
Choi-Sledemki, Yong Mi; Pauls, Heinz W.;
Barton, Jeffrey N.; Ewing, William R.; Green, Daniel
M.; Becker, Michael R.; Gong, Yong; Levell, Julian
Aventis Pharma Deutschland G.m.b.H., Germany
PCT Int. Appl., 106 pp.
CODEN: PIXXD2
Patent

US 1998-90492

A2 19980603

PATENT ASSIGNEE(S):

Patent English

PA'	PATENT NO.						DATE			APPI	LICAT	ION :	NO.		D.	ATE	
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	2001									wo :	2000-	EP11	577		2	0001	121
WO	2001	0397	59		A3		2002	0117									
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	RW:										, TZ,						
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											, MR,						
US	6281	227			B1		2001	0828	1	US :	1999 -	4533	07		1	9991	202
PRIORIT	Y APP	LN	INFO	. :					1	US 1	1999-	4533	07		A 1	9991	202
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									1	US 1	1998 -	90492	2	- 2	A2 1	9980	603
									1	WO 1	1999-1	JS12:	312		12 1	9990	603

OTHER SOURCE(S): MARPAT 135:46082

Title compds. [(un)substituted I; R = N-containing heteroaryl; R1 = H, (acyl)alkyl, (hetero)arylalkyl, etc.; R2 = H, (hetero)arylalkyl, carbamoylalkyl, etc.; Z = (NH- or NHCO-interrupted or -terminated) alkylene; Z1 = (CH2)0-3] were prepared Thus, I (R1 = H, Z1 = CH2)(II; R

L10 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

H, R2 = CO2CMe3, Z = bond) was N-alkylated by 7-bromomethyl-1chloroisoquinoline (prepn. each given) and the deprotected product
N-acylated by 7-methoxynaphthalene-2-sulfonyl chloride (prepn. given) to
give, in 2 addnl. steps, II (R = 1-amino-7-isoquinolyl, R2 =
7-methoxynaphthalene-2-sulfonyl, Z = CH2). Data for biol. activity of I
were given.

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LIO ANSWER 5 OF 7
ACCESSION NUMBER:
DOCUMENT NUMBER:
133:144473
Solid-phase parallel synthesis of azarene
pyrrolidinones as factor Xa inhibitors
Gong, Yong, Becker, Michael; Choi-Sledeski, Yong
Ni; Davis, Roderick S.; Salvino, Joseph M.; Chu,
Valeria; Brown, Karen D.; Pauls, Henry W.

CORPORATE SOURCE:
DEPARTMENT OF THE SOURCE:
SOURCE:
Bioorganic & Medicinal Chemistry, Rhone-Poulenc
Rorer, Collegeville, PA, 19426, USA
Bioorganic & Medicinal Chemistry Letters (2000),
10(10), 1033-1036
CODEN: BMCLES; ISSN: 0960-894X
Elsevier Science Ltd.
Journal
PUBLISHER:
DOCUMENT TYPE:
LANGUAGE:
OTHER SOURCE(S):
GI
                                                                                                                                                  English
CASREACT 133:144473
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A focused library (4+14) prepared from 4-aminopyridine and 4-, 5-, and 6-azoindole templates was synthesized using 14 polymer-supported 4-amido-2,3.5.6-tetrafluorophenyl (TFP) sulfonate esters and heteroarylmethyl-substituted arylsulfonylamino pyrrolidinones such as I

give a library of factor Xa inhibitors such as II. Several compds. were identified as factor Xa inhibitors (IC50≤0.1 µM) helping to establish the SAR among these four series of azarene pyrrolidinones. E.g., factor Xa was inhibited by II with a Ki of 15 nM. MENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

E.g., facto REFERENCE COUNT: THIS

FORMAT

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L10 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2000:543073 CAPLUS DOCUMENT NUMBER: 133:261091
  TITLE:
                                                                      Crystal Structures of Human Factor Xa Complexed with
                                                                       Potent Inhibitors
                                                                      Maignan, Sebastien; Guilloteau, Jean-Pierre;
  AUTHOR (S) :
  Pouzieux.
                                                                      Stephanie; Choi-Sledeski, Yong Mi; Becker,
Michael R.; Klein, Scott I.; Ewing, William R.;
 Pauls.
                                                                     Henry W.; Spada, Alfred P.; Mikol, Vincent
Department of Structural Biology, Aventie Pharma,
Vitry/Seine, F.94403, Fr.
Journal of Medicinal Chemistry (2000), 43(17),
3226-3232
 CORPORATE SOURCE:
 SOURCE:
                                                                      CODEN: JMCMAR; ISSN: 0022-2623
American Chemical Society
  PUBLISHER:
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Involved in the coagulation cascade, factor Xa (FXa) is a serine protease
which has received great interest as a potential target for the
development of new antithrombotics. Although there is a great wealth of
structural data on thrombin complexes, few structures of ligand/FXa
complexes have been reported, presumably because of the difficulty in
growing crystals. Reproducible crystallization conditions for human
des-clai-45
              Slai-45 coagulation FXs have been found. This has led to an improvement in the diffraction quality of the crystals (about 2.1 Å) when compared to the previously reported forms (2.3-2.8 Å) thus providing a suitable platform for a structure-based drug design approach. A series of crystal structures of noncovalent inhibitors complexed with FXs have been remined.
               three of which are presented herein. These include compds. containing
 benzamidine moiety and surrogates of the basic group. The
benzamidine-containing compound binds in a canonical feshion typical of
synthetic serine protease inhibitors. On the contrary, mols. that
contain
contain
surrogates of the benzamidine group do not make direct hydrogen-bonding
interactions with the carboxylate of Asp189 at the bottom of the S1
pocket. The structural data provide a likely explanation for the
specificity of these inhibitors and a great aid in the design of
bioavailable potent FXa inhibitors.
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR
THIS
                                                                                     RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT
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L10 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:784099 CAPLUS
DOCUMENT NUMBER: 132:22881
TITLE: Sulfonic acid or sulfonylamino N(heteroaralkyl)azaheterocyclic amides as inhibitors factor Xa
Choi-Sledeski, Yong Mi; Pauls, Heinz W.;
Barton, Jeffrey N.; Ewing, William R.; Green, Daniel
M.; Becker, Michael R.; Gong, Yong; Levell, Julian
Rhone-Poulenc Rorer Pharmaceuticals Inc., USA
PCT Int. Appl., 202 pp.
CODEN: PIXXD2
Parent INVENTOR(S): PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English DATENT NO VIND DATE ADDITION NO

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WO 99																
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-										RU,						
K	: GH,															
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115.66	C1,	CM,	GA,	GN,	GW,	ML,	MK,	NE.	SN,	TD,	1G					
US 00	12004			D1		2003	1200		05 1	998-	9049				13380	603
US 66 CA 23 AU 99	12200			AA N1		1999	1203		DII I	000	4333	994			19990	603
AU 33	3642			A1		1222	2220		MU 1	,,,,-	4327	٠.			13330	603
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		FI.		UE,	DK,	E3,	FR,	GB,	GK,		ы.	DO,	м.,	36	,	LE,
BR 99				А		2001	1009		DD 1		1089	٥			10000	603
	25173					2001	0618		TD 2	000-	5521	16			19990 19990	603
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US 62: NO 20	00059	12		Δ.		2001	0131		NO 3	000-	5912	• •			20001	
	20133					2002	0131		us a	000-	9180	3 9			20010	
PRIORITY A									US 1	998-	9049	2		3.2	19980	
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									US 1	996-	3315	9 P		P	19961	213
								,	WO 1	997-1	JS22	406		4.2	19971	203
									WO 1	999-1	JS 12	312	1	N	19990	603
									US 1	999-	1533	07		A3	19991	202

L10 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Aza heterocycles I [X = (CHR3)m; R = (un)substituted heteroaryl; R1, R2 = H, (un)substituted alkyl, alkenyl, aralkyl; R3 = H, OH, (un)substituted alkyl, aryl, heteroaryl; R4 = H, (un)substituted alkyl, aryl, aralkyl; R5,

R6 = H; R5R6 = O; R7, R8 = H, (un)substituted alkyl, aryl, aralkyl, heteroaryl; R7R8 = O; R3R7 = alkylene; m = 0-3) were prepared I are inhibitors of the activity of Factor Xa. Thus, the amide II was prepared from 3-acetamido-4-methylbenzaldehyde, malonic acid, and 7-methoxy-2-naphthalenesulfonyl chloride in 10 steps. II had a Ki of 80 nM for inhibition of factor Xa.

RENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L10 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) WO 1999-US12312 A2 19990603

OTHER SOURCE(S):

MARPAT 129:81744

The compds. of formula [I; Arl * a bicyclic heteroaryl containing ≥ 1 N atom; Z = alkenyl; Rl = H, (un)substituted alkyl, aralkyl, or heteroalkyl,

heteroalkyl,
hydroxyalkyl, carboxy alkyl, carbamoylalkyl, aminoalkyl, etc.; R2 =
R35(O)p, R3R4NS(O)p; R3. = (un)substituted alkyl, cycloalkyl,
heterocyclyl,
aryl, heteroaryl, aralkyl, heteroaralkyl, aralkenyl, heteroaralkenyl; or
R1 and R3 taken together with N(O)p or NS(O)pNR4 through which R1 and R3
are linked from a 5 to 7 membered (un)substituted heterocyclyl; wherein p
= 1, 2; R4 = (un)substituted alkyl, cycloalkyl, heterocyclyl, aryl,
heteroaryl, etc.; X1, X1a = H, (un)substituted alkyl, aryl, aralkyl,
heteroaryl, or heteroaralkyl; or X and X1a are taken together to form
oxo:

II

X3 = H, OH, (un) substituted alkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl; or X3 or one of X1 and X1a taken together form a 4 to 7 membered cycloalkyl; X5, X5a, X5b = H, (un) substituted NH2. HONH, alkoxyamino, NHNH2, (un) substituted OH, CONH2 or SO2NH2, halo, cyano,

etc.; one of X5, X5a, and X5a = H, HO or (H, optionally substituted lower alkyl, hydroxy, alkoxy, or amino)NH that substitutes the distal ring of Arl at a position alpha to a nitrogen thereof) herein exhibit useful

Prepared by: Mary Hale @2-2507 Rem Bldq 1D86

L10 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 1998:402310 CAPLUS DOCUMENT NUMBER: 129:81744

TITLE:

129:81744
Preparation of sulfonic acid or sulfonylamino
N-(heteroaralkyl)-azaheterocyclylamide compounds as inhibitors of factor Xa
Choi-Sledaski, Yong Mi; Pauls, Henry W.;
Barton, Jeffrey N.; Ewing, William R.; Green, Daniel M.; Becker, Michael R.; et al.
Rhone-Poulenc Rorer Pharmaceuticals Inc., USA
PCT Int. Appl., 116 pp.
CODEN: PIXXD2
Patent

INVENTOR(S):

PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT	INFOR	MATI	ON:																
PA:	rent .	NO.			KIN	Þ	DATE			API	LIC	AT I	ON	NO.			DA	TE	
WO	9825				A1		1998	0618		WO	199	7-1	JS22	406			19	971	203
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		GN,	ML,	MR,	NE,	SN,	TD,	TG											
CA.	2274 9855	686			AA		1998	0618		CA	199	7-2	274	586			19	971:	203
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AU	7266	37			B2		2000	1116											
EP	9443 9443	36			Al		1999	0929		EP	199	7-5	515	73			19	971	203
EP	9443	36		-	- 81		2002	0918			_	_							
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CN DD	1244 9713	790			^		2000	0216		CN	199	7-1	8138	37				971:	
7.0	2001	257			A ma		20001	321		BK	199	7-1	392				19	971:	203
3.0	1032	5000.	30		12		2001	5522		J P	199	8-5	2684	14					
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24	97112	207			A .		1000	7720		73	100	7-9	212	, ,			19	9712 9712 9712	203
IIS	66028	364			B1		2002	200		UC.	133	,- <u>1</u>	0401						
NO	9902	353			A		1999	1810		NO.	100	0-3	0492	•			19	9806	
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US	6281	227			B1		2001	1828		ITC	100	0-4	E220	77			19:	3306	111
US	20021	31331	0.0		Al		20021	1121		170	200	1 - 0	1007	,,			7 A .	3312	202
PRIORITY	APP	IN.	NFO	. :			20020	,,,,		115	100	6.2	2150	20		,	10	010	130
	99028 31243 20000 62813 20020												0.200		,		19:	3012	.13
									•	WO	199	7 - U	S224	06	P	J	19	9712	03
						•				US	199	8 - 9	0492	3	7	.2	19	9806	03

ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) pharmacol. activity and accordingly are incorporated into pharmaceutical compns. and used in the treatment of patients suffering from certain medical disorders. More specifically, they are inhibitors of the vity

activity
of Factor Xa. The present invention is directed to compds. of formula I,
compns. contgs. compds. of formula I, and their use, which are for

ting a patient suffering from, or subject to, physiol. condition (disorder) which can be ameliorated by the administration of an inhibitor of the activity of Pactor Xa. The physiol. disorder is venous vasculature, arterial vasculature, abnormal thrombus formation, acute myocardial infarction, unstable angina, thromboembolism, acute vessel closure

with thrombolytic therapy, percutaneous transluminal coronary

angioplasty,
transient ischemic attacks, stroke, intermittent claudication or bypass
grafting of the coronary or peripheral arteries, vessel luminal

grafting of the coronary or perspects associately, maintenance of vascular arrowing, restenosis post-coronary or venous angioplasty, maintenance of vascular access patency in long-term hemodialysis patients, pathol. Thrombus formation occurring in the veins of the lower extremities following abdominal, knee and hip surgery, a risk of pulmonary thromboembolism, or disseminated systemic intravascular coagulopathy occurring in vascular systems during septic shock, certain viral infections and cancer. Thus, 3-(S)-smino-1-(6-amino-1-chloroisoquinolin-7-ylmethyl)pyrrolidin-2-one was

was

coupled with 7-methoxynaphthalene-2-sulfonyl chloride followed by amination with ammonium acetate in PhOH at 115° for 2 h gave the title compd.,

N-[N-(isoquinolinylmethyl)oxopyrrolidinyl]naphthalenesulfona mide (II.CF3CO2H). II.CF3CO2H in vitro inhibited factor Xa. thrombin, trypein, tissue-plasminogen activator (t-PA), plasmin and activated protein C with Ki value of 80 nM.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS FORMAT

FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

=> log y COST IN U.S. DOLLARS

SINCE FILE TENTRY SES

TOTAL SESSION

FULL ESTIMATED COST

145.44

478.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

CA SUBSCRIBER PRICE

ENTRY -18.98 SESSION -18.98

STN INTERNATIONAL LOGOFF AT 10:02:51 ON 23 JUN 2005

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